Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information for:

^{45}Sc Solid-State NMR Studies of $Cp^*_2Sc–X$ and $Cp^*_2ScX(THF)$

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Solution ^{45}Sc NMRs of Cp*$_2$ScX.

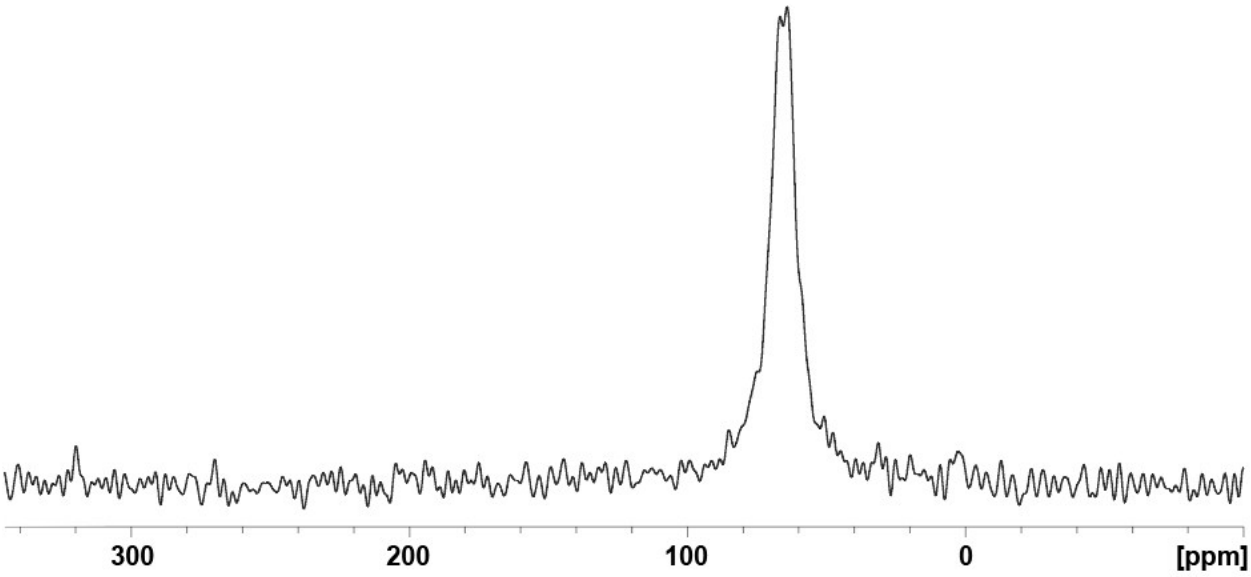


Figure S1. ^{45}Sc{^{1}H} NMR of Cp*$_2$ScF in C_6D_6**,** ns = 1024 and d1 = 0.05 sec**.**

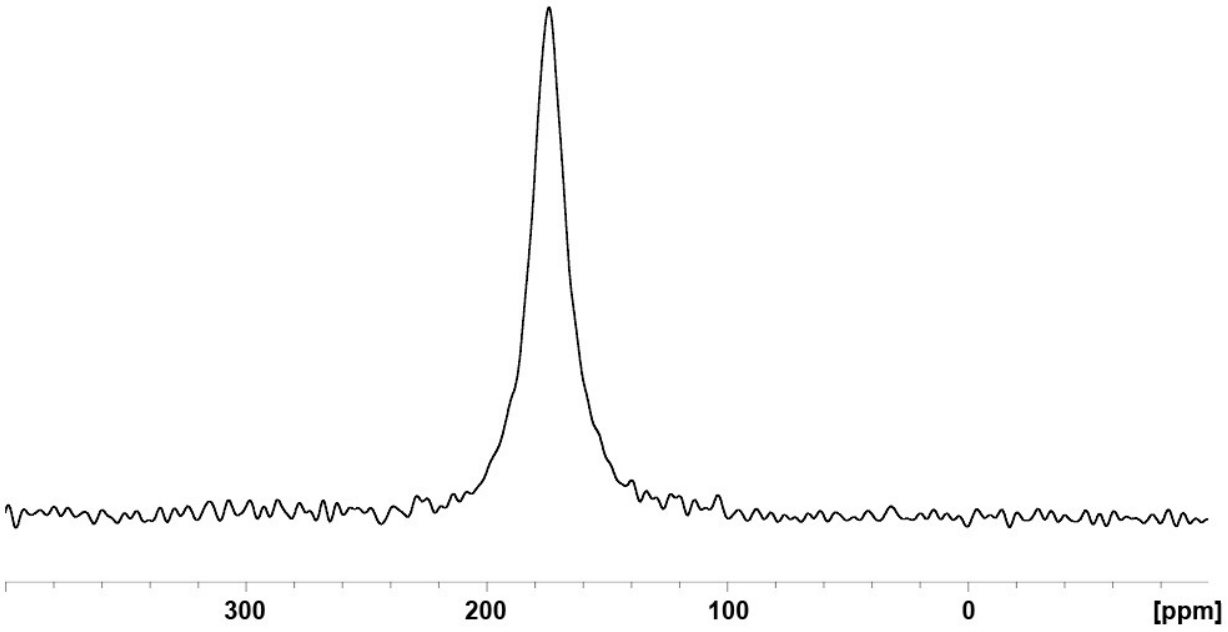


Figure S2. ^{45}Sc{^{1}H} NMR of Cp*$_2$ScCl in C_6D_6**,** ns = 1024 and d1 = 0.05 sec**.**

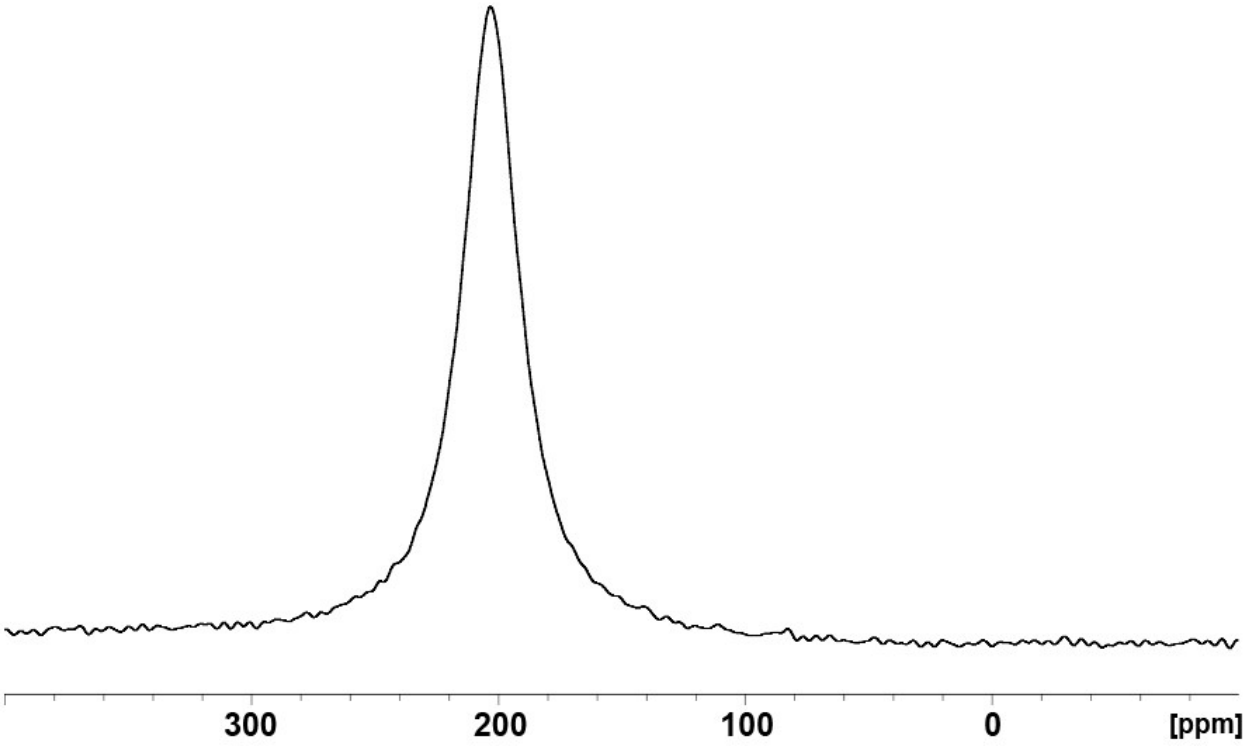


Figure S3. $^{45}Sc\{^{1}H\}$ NMR of Cp^*_2ScBr in C_6D_6, ns = 1024 and d1 = 0.05 sec.

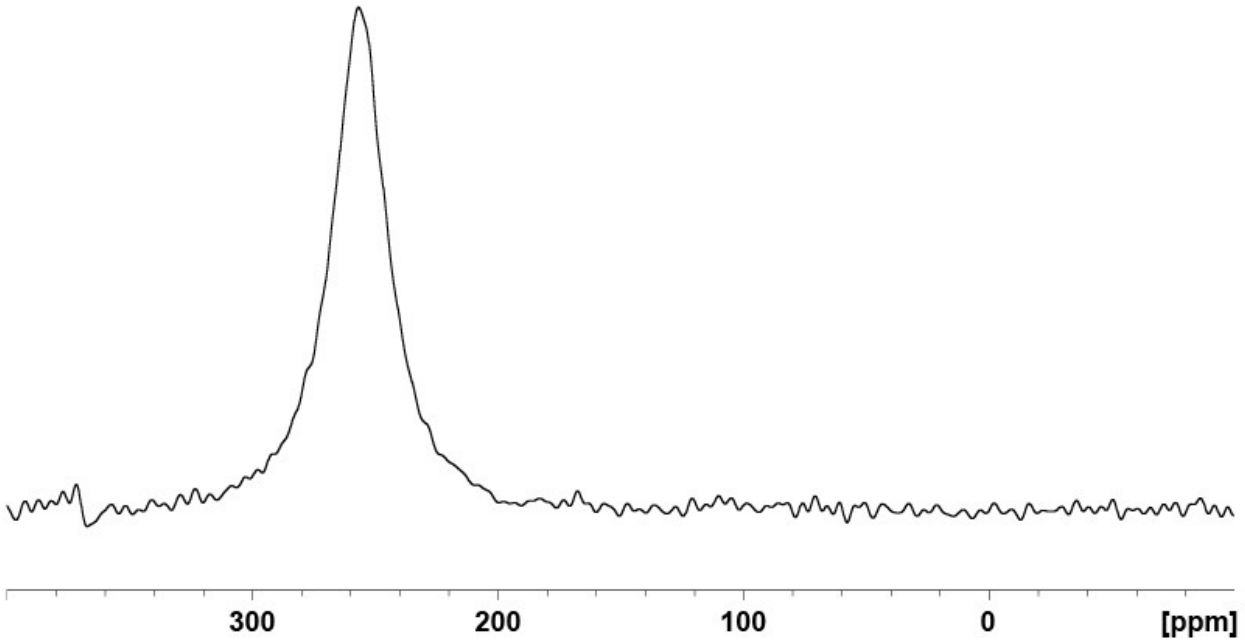


Figure S4. $^{45}Sc\{^{1}H\}$ NMR of Cp^*_2ScI in C_6D_6, ns = 1024 and d1 = 0.05 sec.

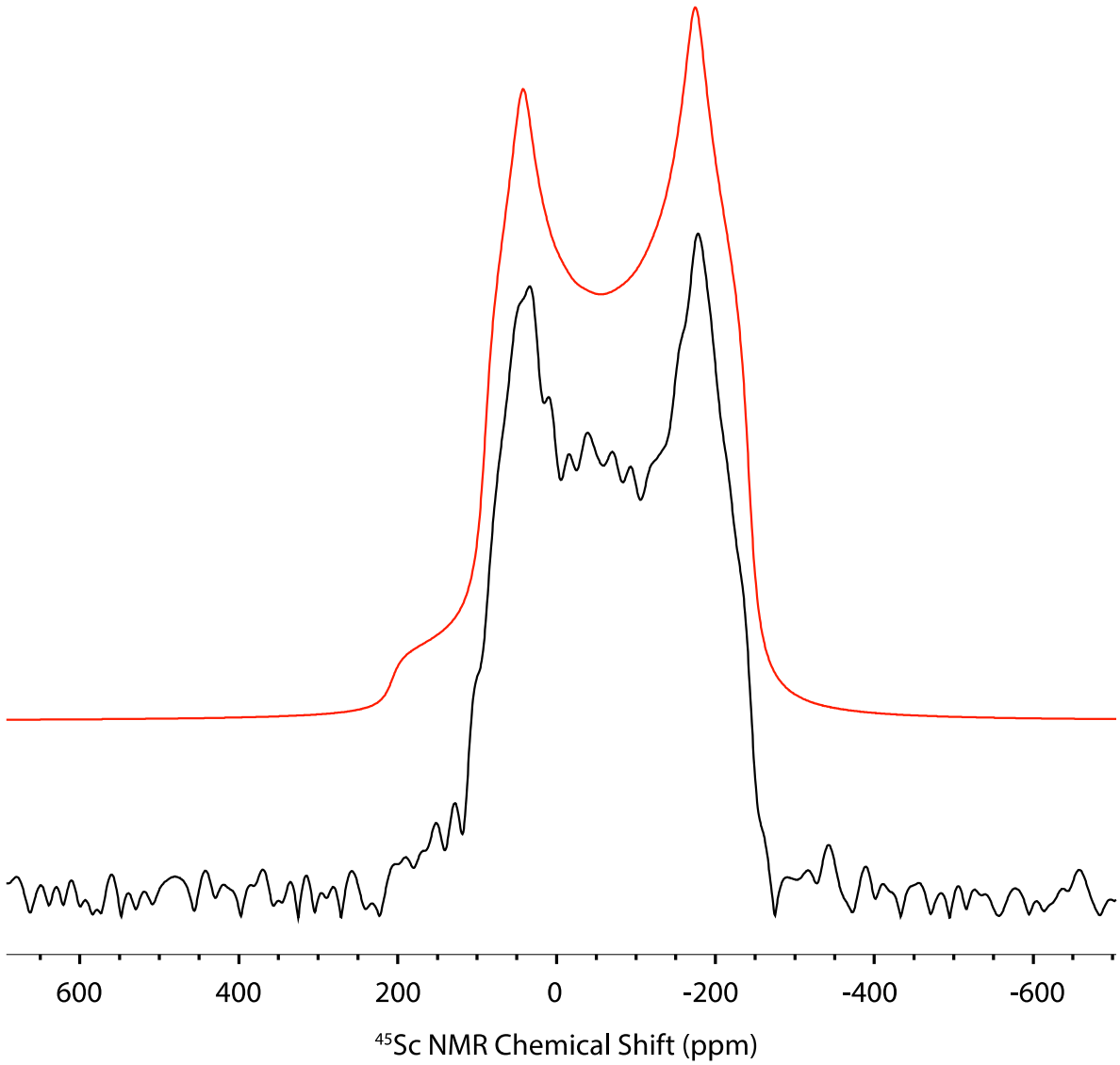


Figure S5. Solid-State ^{45}Sc NMR of Cp*$_2$ScF(THF) (black) with a simulated spectrum (red).

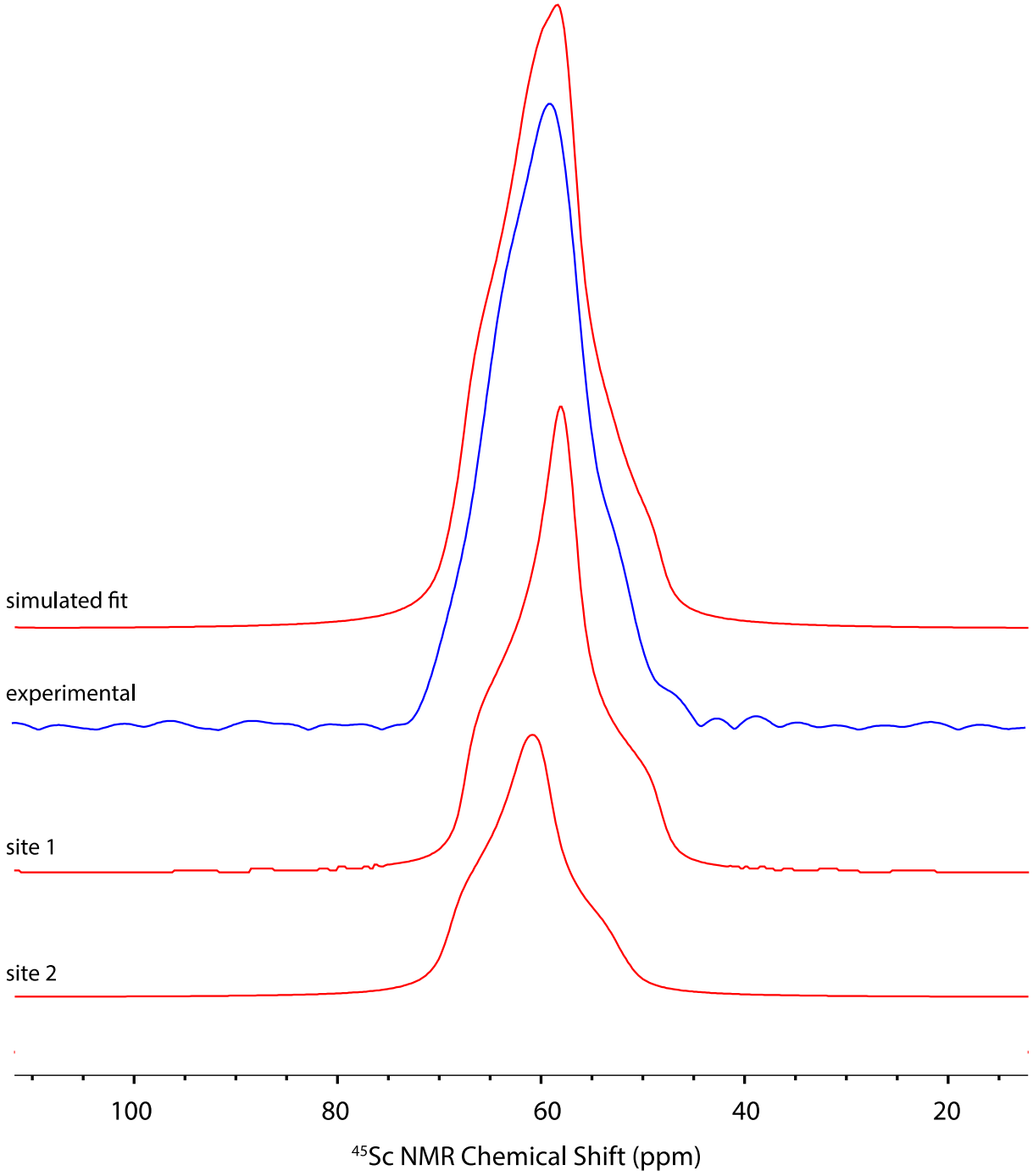


Figure S6. ^{45}Sc 1D MAS echo spectrum of Cp*$_2$ScCl(THF) at 14.1 T spinning at 9 kHz (blue). The simulated fit is shown above the experimental spectrum using values obtained from the MQMAS experiment shown in Figure 3 of the main text. Each site is shown below the experimental spectrum. Removal of any one site results in a lower quality simulated spectrum than shown in the figure.

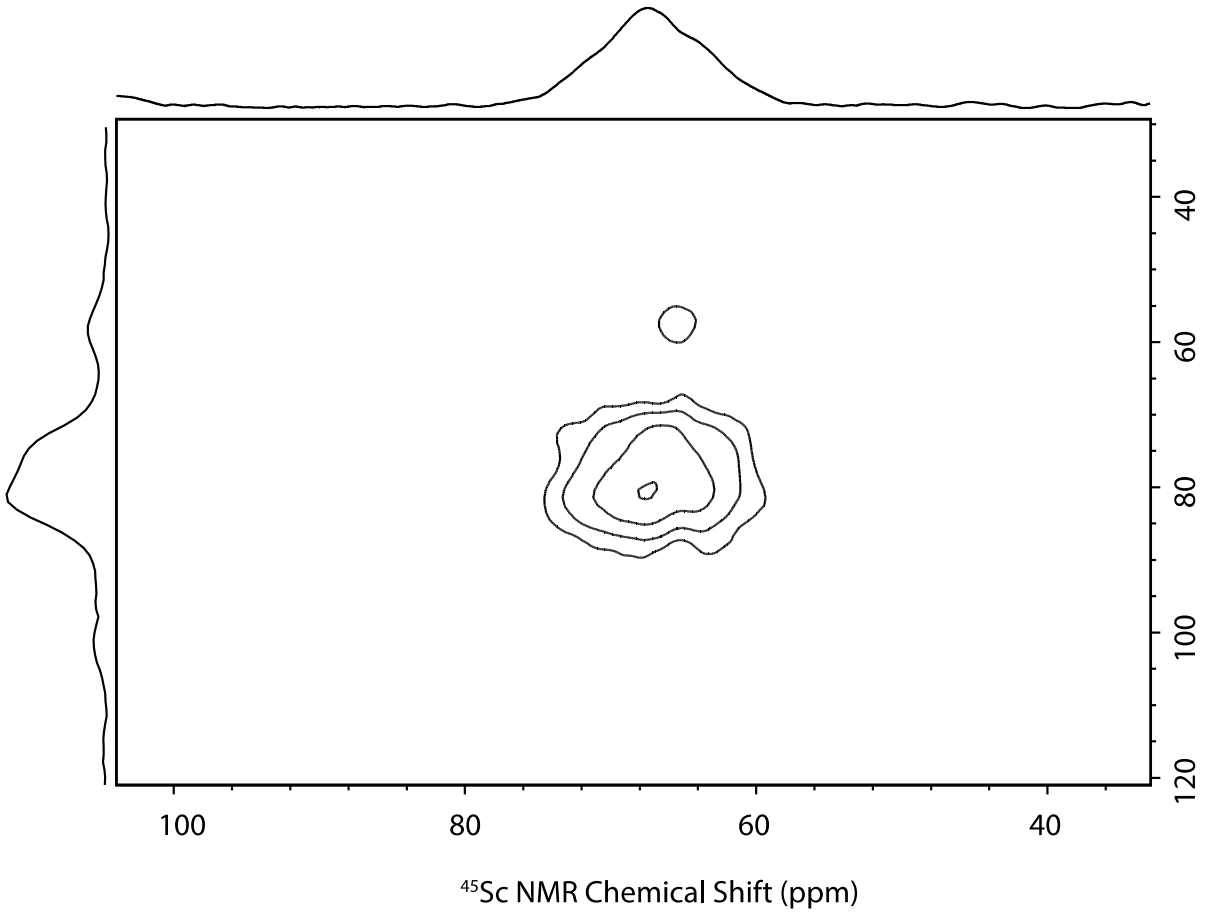


Figure S7. ^{45}Sc 3QMAS NMR of Cp*$_2$ScCl(THF) at 9.4 T. The spectrum contains similar information as the spectrum shown in Figure 3, though with lower resolution because of the lower magnetic field in this experiment.

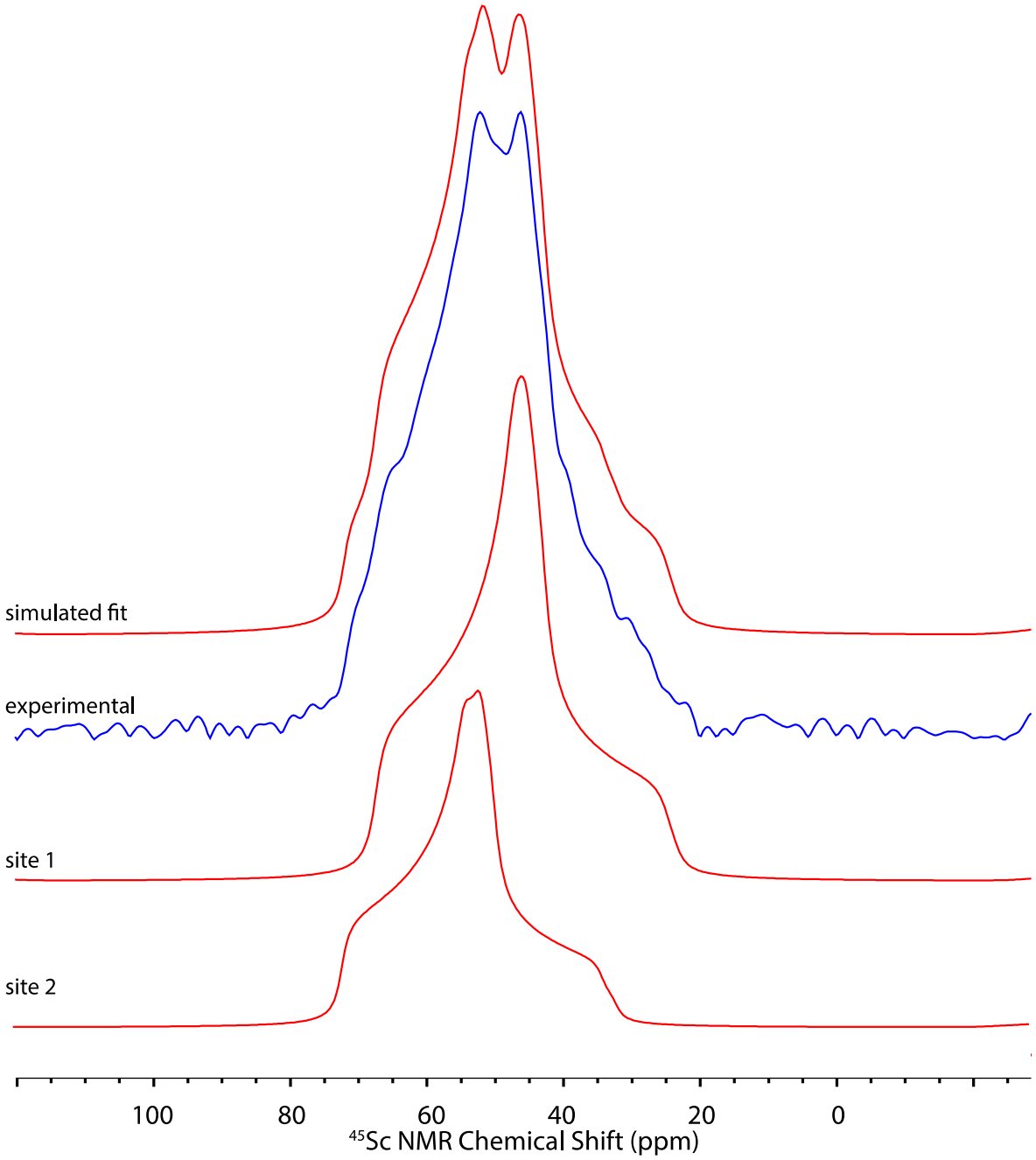


Figure S8. ^{45}Sc 1D MAS echo spectrum of Cp*$_2$ScCl(THF) at 9.4 T spinning at 9 kHz (blue). The simulated fit is shown above the experimental spectrum using values obtained from the MQMAS experiment shown in Figure 3 of the main text. Each site is shown below the experimental spectrum. Removal of any one site results in a lower quality simulated spectrum than shown in the figure.

Table S1. Summary of NMR Data for $Cp^*_2ScCl(THF)$

	MAS (14.1 T)		MAS (9.4 T)	
δ_{iso} (ppm)	68	70	68	72
C_Q (MHz)	7.5	7.3	7.5	7.2
η	0.9	0.8	0.9	0.8

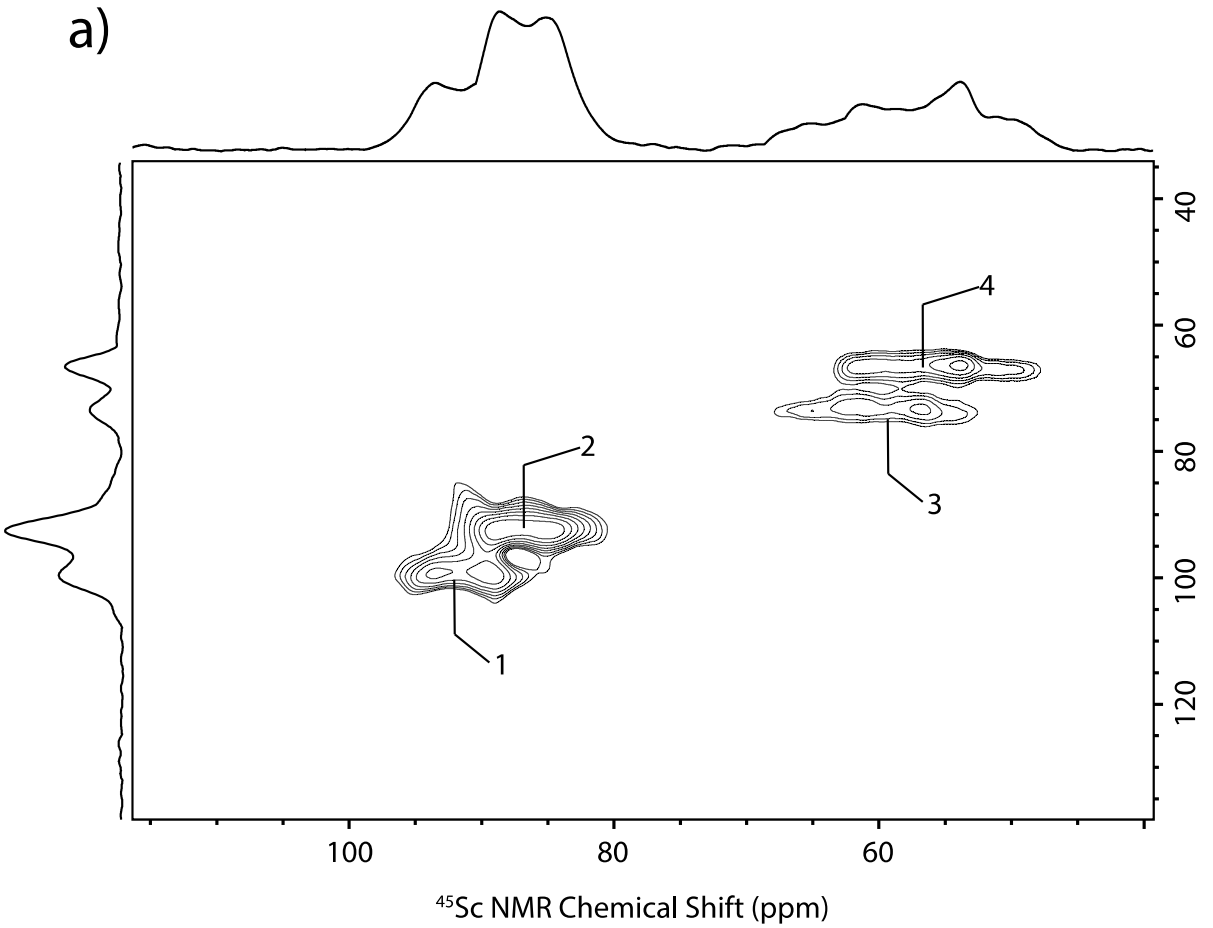


Figure S9. ^{45}Sc 3QMAS NMR of Cp*$_2$ScBr(THF) at 14.1 T.

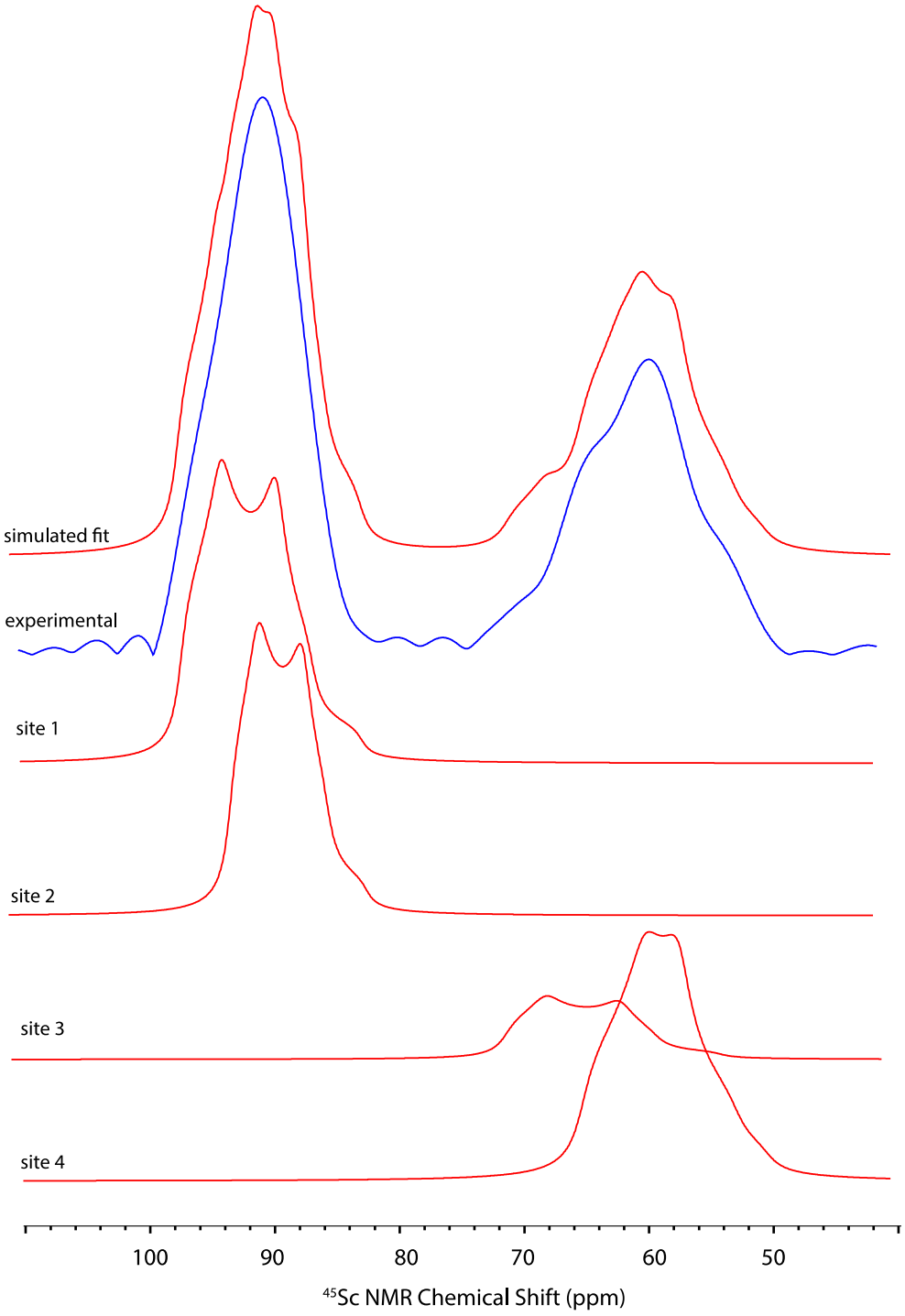


Figure S10. ^{45}Sc 1D MAS echo spectrum of Cp*$_2$ScBr(THF) at 14.1 T spinning at 9 kHz (blue). The simulated fit is shown above the experimental spectrum using values obtained from the MQMAS experiment shown in Figure S9. Each site is shown below the experimental spectrum.

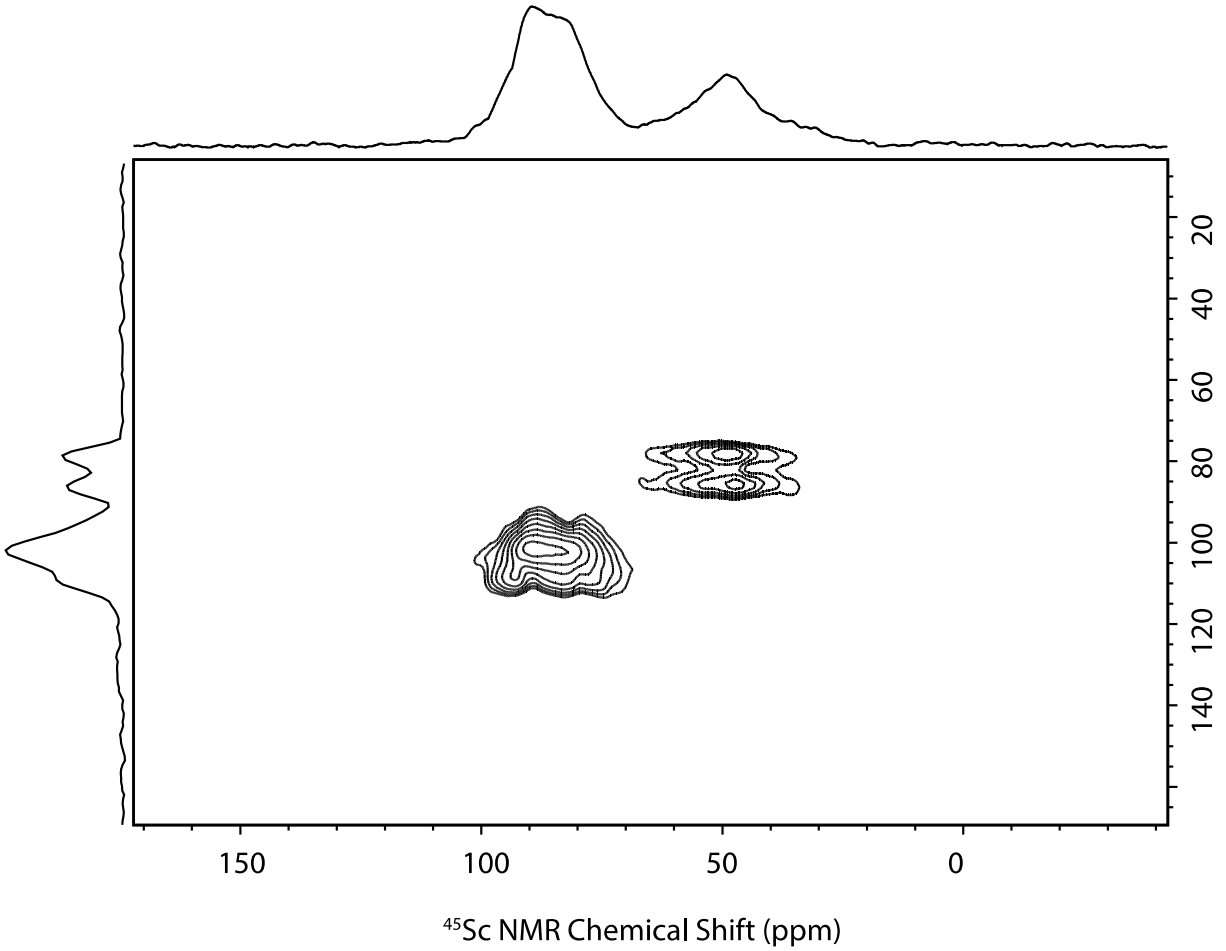


Figure S11. ^{45}Sc 3QMAS NMR of Cp*$_2$ScBr(THF) at 9.4 T. The spectrum contains similar information as the spectrum shown in Figure S9, though with lower resolution because of the lower applied magnetic field in this experiment.

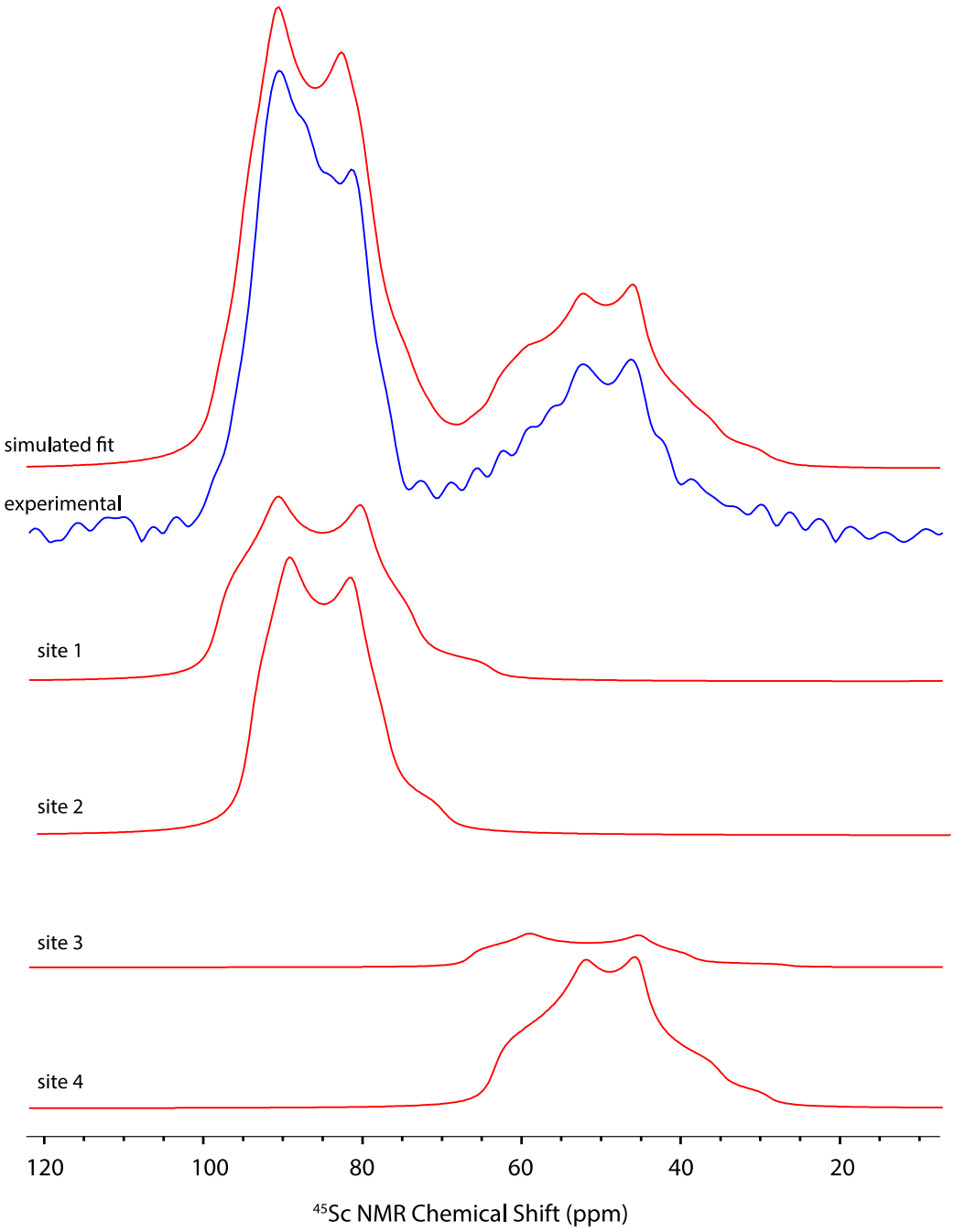


Figure S12. ^{45}Sc 1D MAS echo spectrum of Cp*$_2$ScBr(THF) at 9.4 T spinning at 9 kHz (blue). The simulated fit is shown above the experimental spectrum using values obtained from the MQMAS experiment shown in Figure S10. Each site is shown below the experimental spectrum.

Table S2. Summary of NMR Data for $Cp^*_2ScBr(THF)$

	MAS (14.1 T)				MAS (9.4 T)			
δ_{iso} (ppm)	98	94	68	63	99	96	69	64
C_Q (MHz)	7.2	6.2	7.9	7.0	7.2	6.2	7.9	7.0
η	0.4	0.3	0.3	0.6	0.4	0.3	0.3	0.6

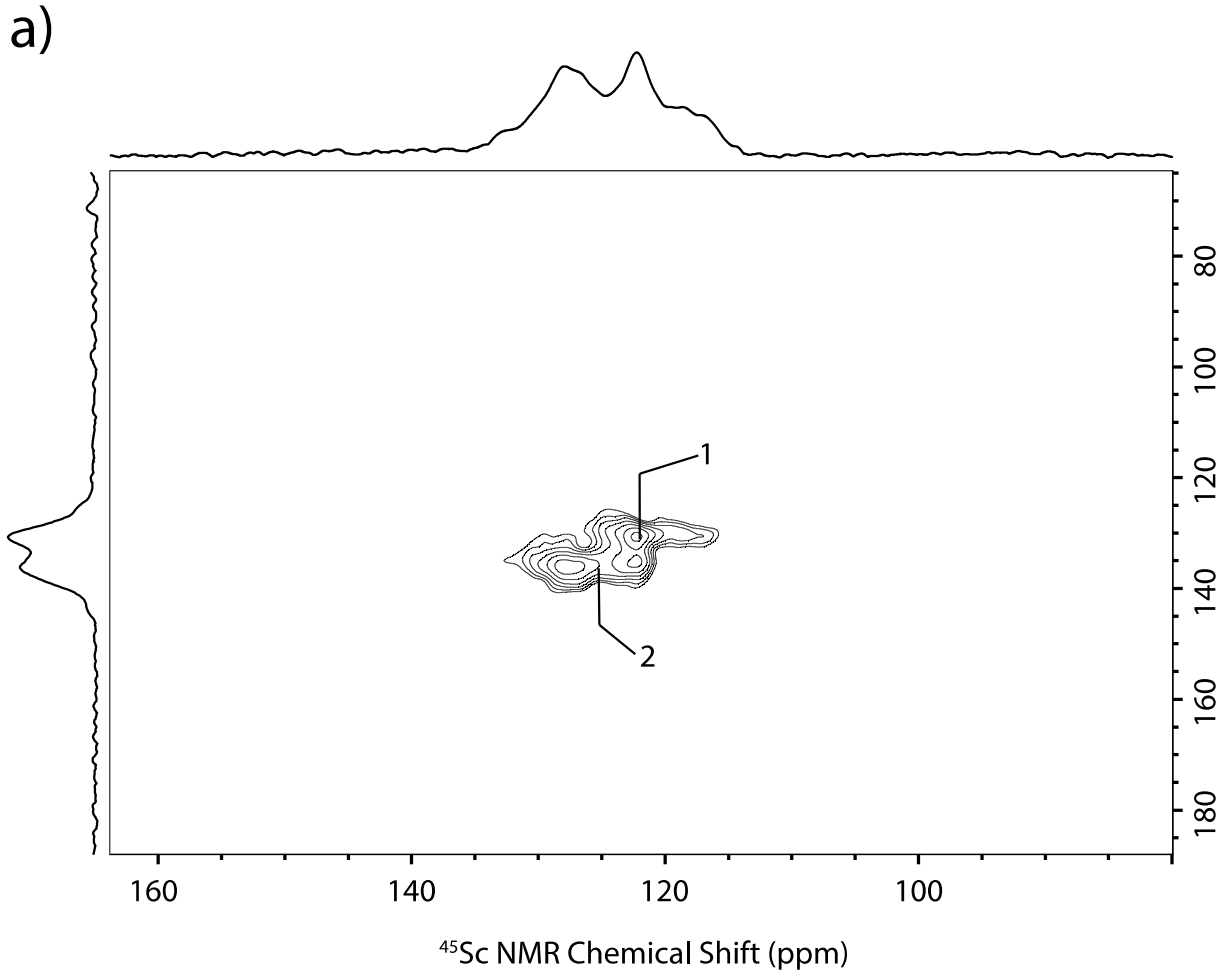


Figure S13. ^{45}Sc 3QMAS NMR of Cp*$_2$ScI(THF) at 14.1 T (a).

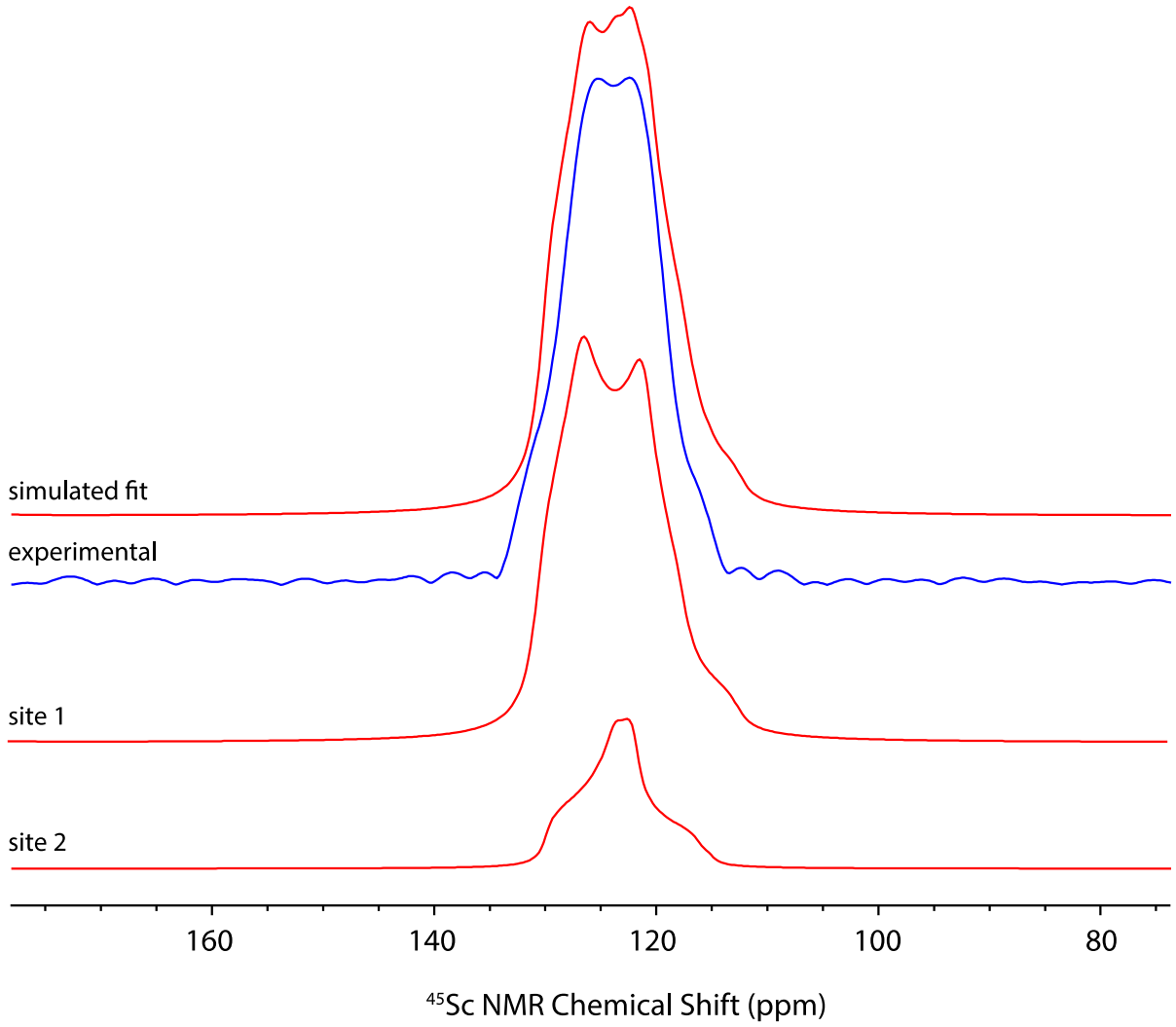


Figure S14. ^{45}Sc 1D MAS echo spectrum of Cp*$_2$ScI(THF) at 14.1 T spinning at 9 kHz (blue). The simulated fit is shown above the experimental spectrum using values obtained from the MQMAS experiment shown in Figure S14. Each site is shown below the experimental spectrum. Removal of any one site results in a lower quality simulated spectrum than shown in the figure.

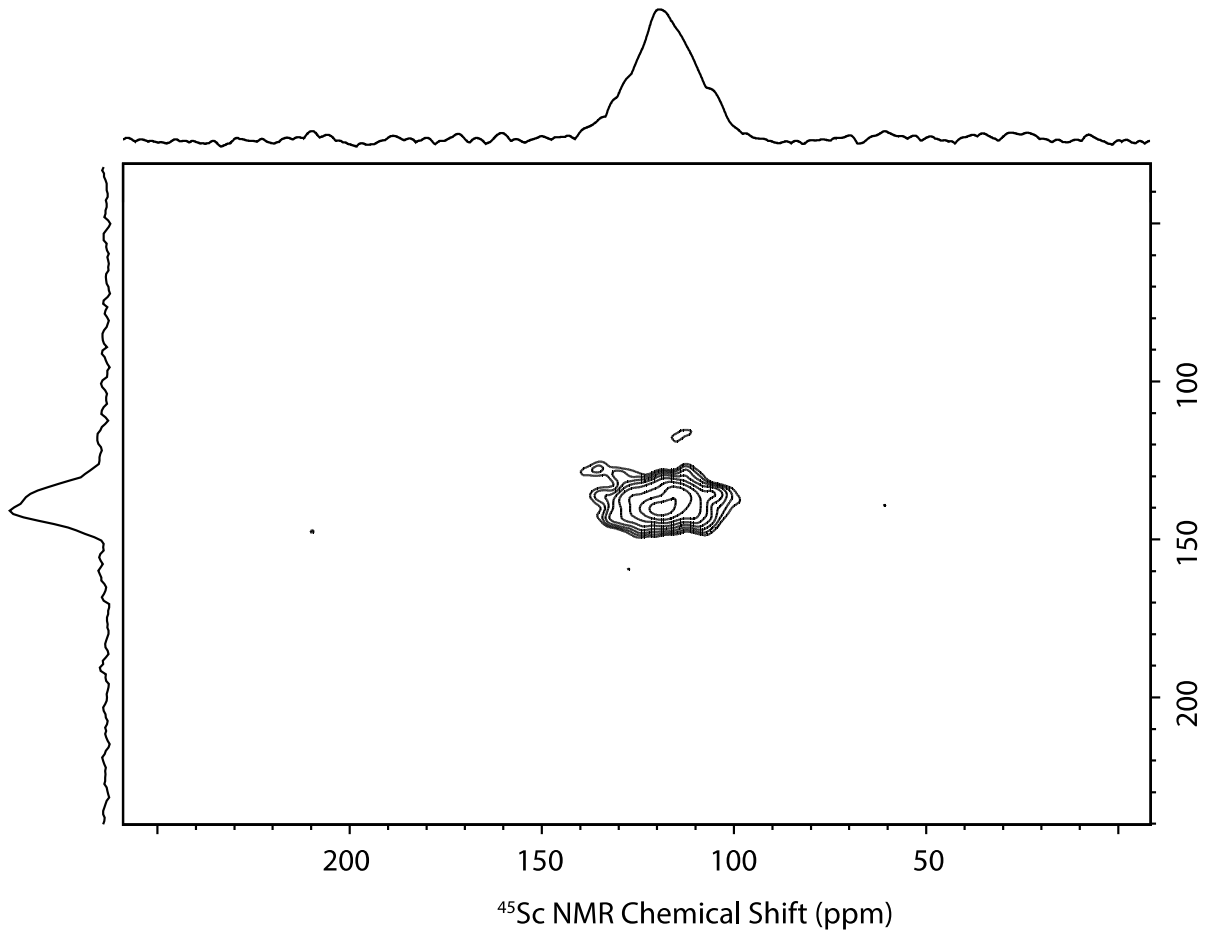


Figure S15. ^{45}Sc 3QMAS NMR of $Cp^*_2ScI(THF)$ at 9.4 T. The spectrum contains similar information as the spectrum shown in Figure S14, though with lower resolution because of the lower applied magnetic field in this experiment.

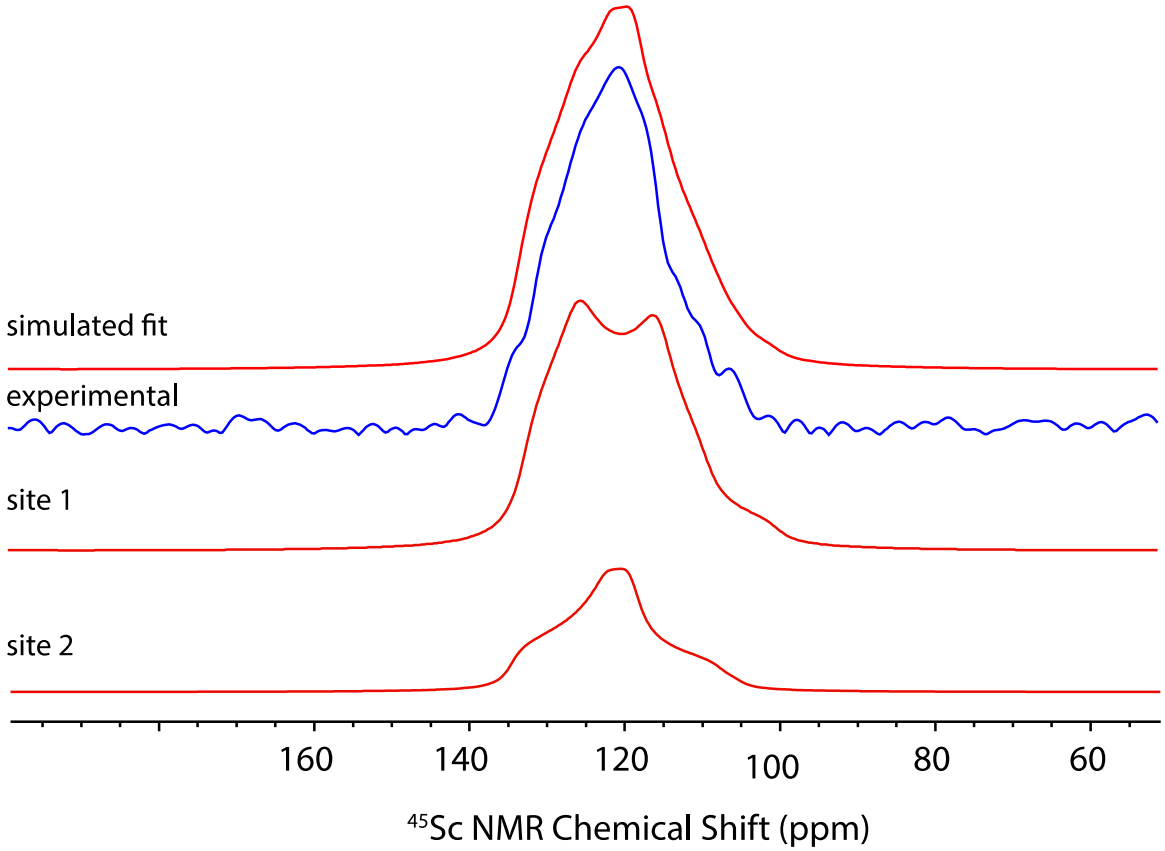


Figure S16. ^{45}Sc 1D MAS echo spectrum of Cp*$_2$ScI(THF) at 9.4 T spinning at 9 kHz (blue). The simulated fit is shown above the experimental spectrum using values obtained from the MQMAS experiment shown in Figure S14. Each site is shown below the experimental spectrum. Removal of any one site results in a lower quality simulated spectrum than shown in the figure.

Table S3. Summary of NMR Data for Cp*$_2$ScI(THF)

	MAS (14.1 T)		**MAS (9.4 T)**	
δ_{iso} (ppm)	128	132	128	132
C_Q (MHz)	6.7	7.8	6.1	7.3
η	0.3	0.8	0.3	0.8

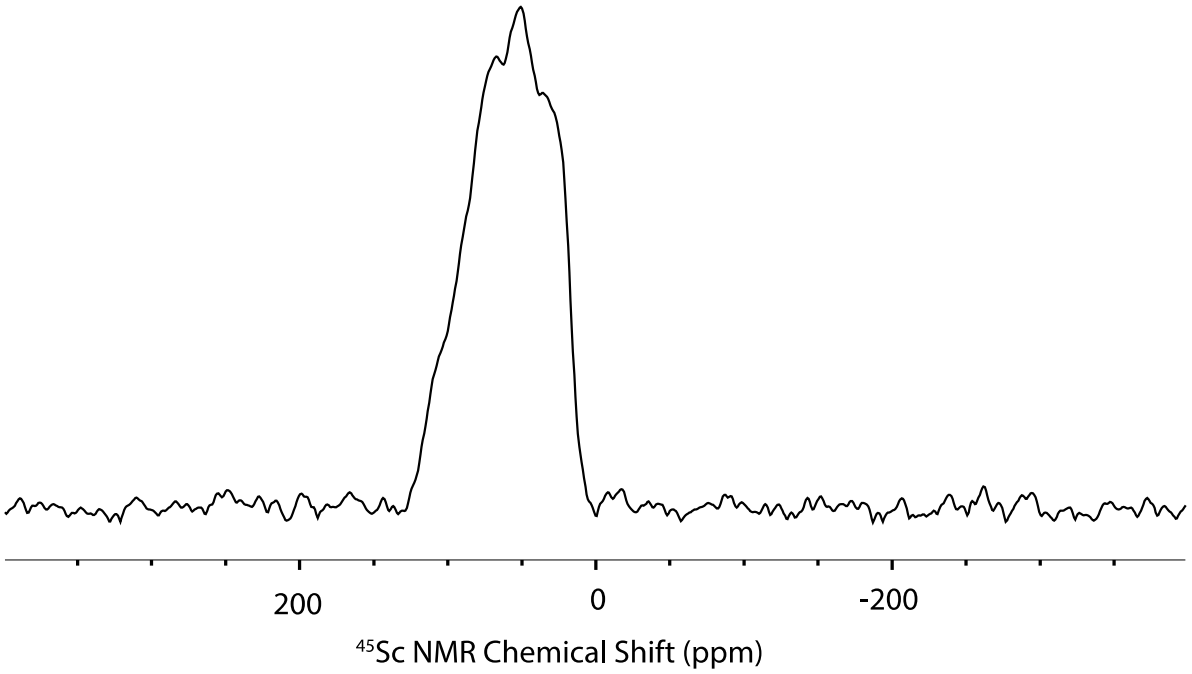


Figure S17. Static ^{45}Sc NMR spectrum of Cp*$_2$ScCl(THF) at 14.1 T.

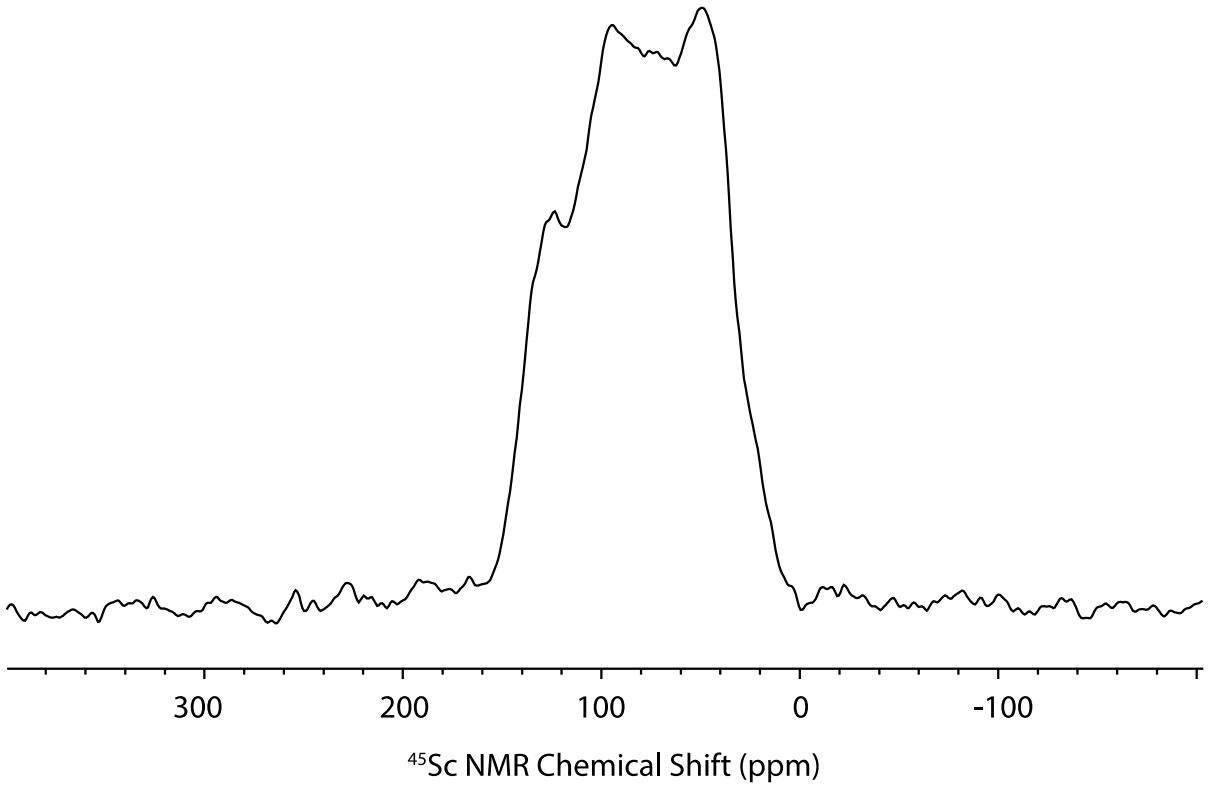


Figure S18. Static ^{45}Sc NMR spectrum of Cp*$_2$ScBr(THF) at 14.1 T.

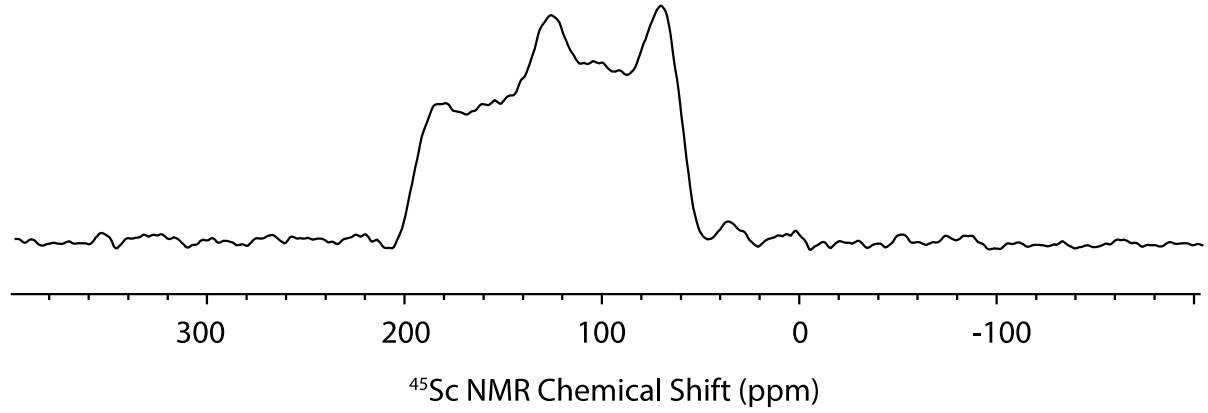


Figure S19. Static ^{45}Sc NMR spectrum of Cp*$_2$ScI(THF) at 14.1 T.

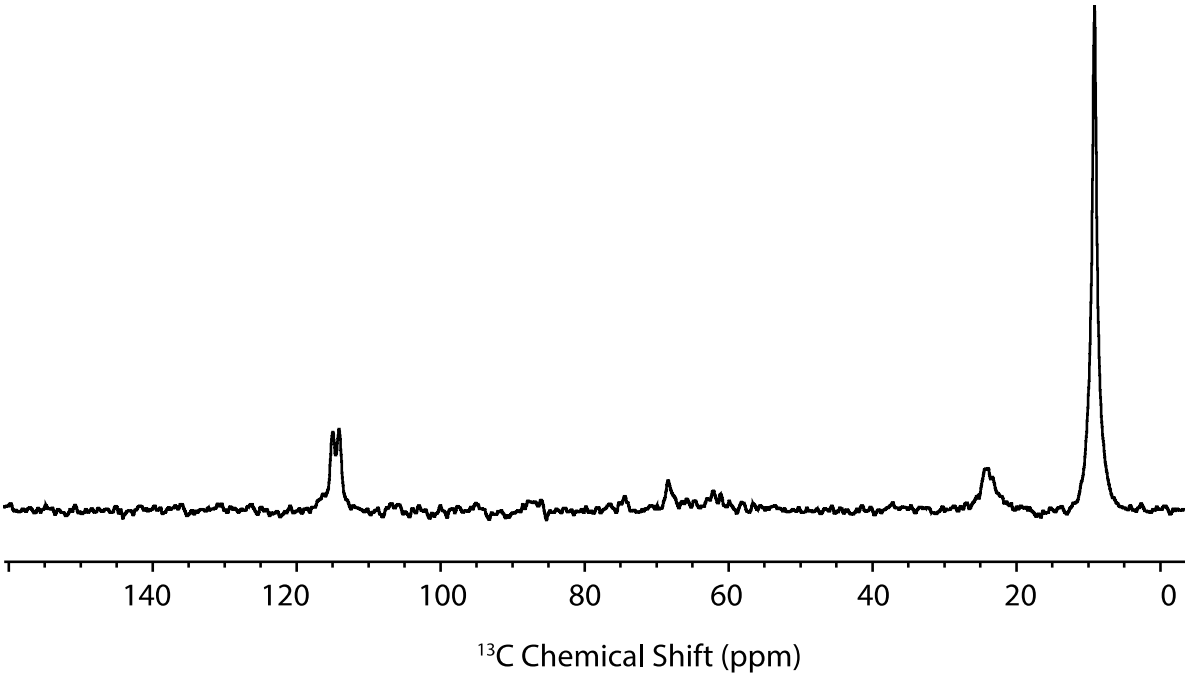


Figure S20. $^{13}C\{^{1}H\}$ CPMAS NMR spectrum of $Cp^*_2Sc–F$ at 10 kHz spinning speed (contact time = 2 ms; * = spinning sideband).

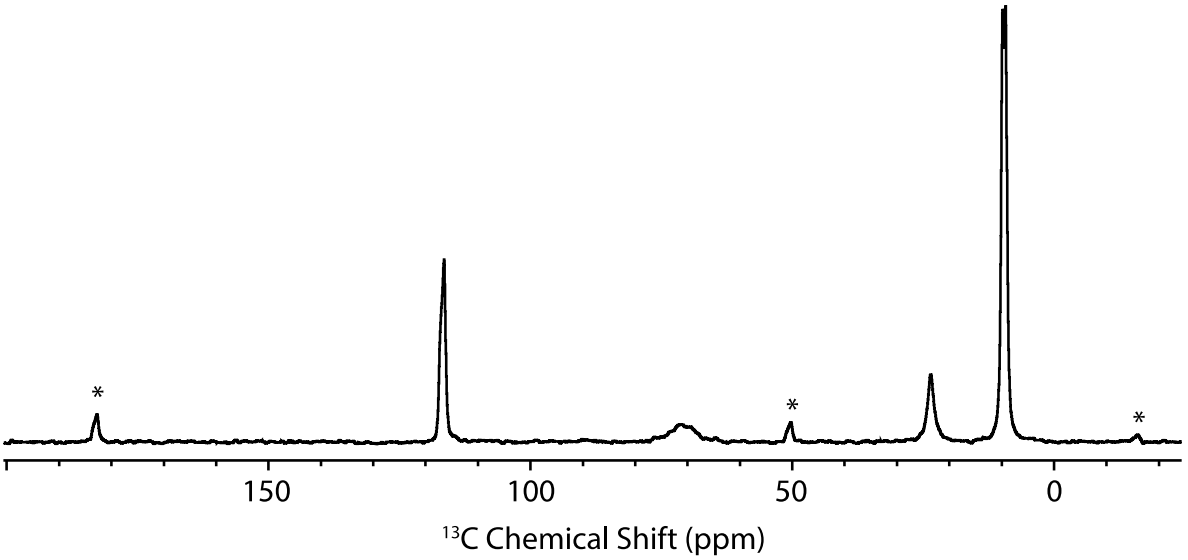


Figure S21. $^{13}C\{^{1}H\}$ CPMAS NMR spectrum of $Cp^*_2Sc–Cl$ at 10 kHz spinning speed (contact time = 2 ms; * = spinning sideband).

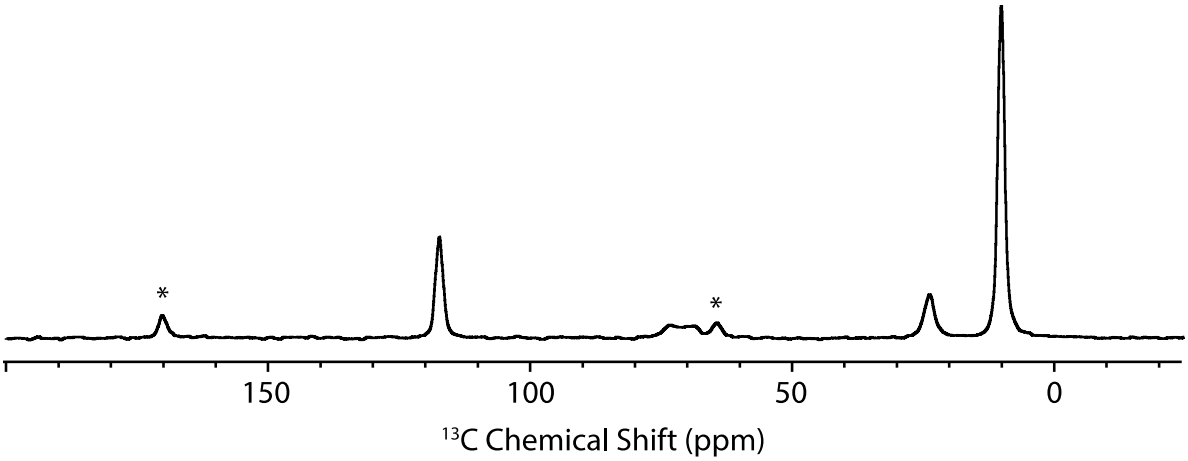


Figure S22. $^{13}C\{^{1}H\}$ CPMAS NMR spectrum of $Cp^*_2Sc–Br$ at 9 kHz spinning speed (contact time = 2 ms; * = spinning sideband).

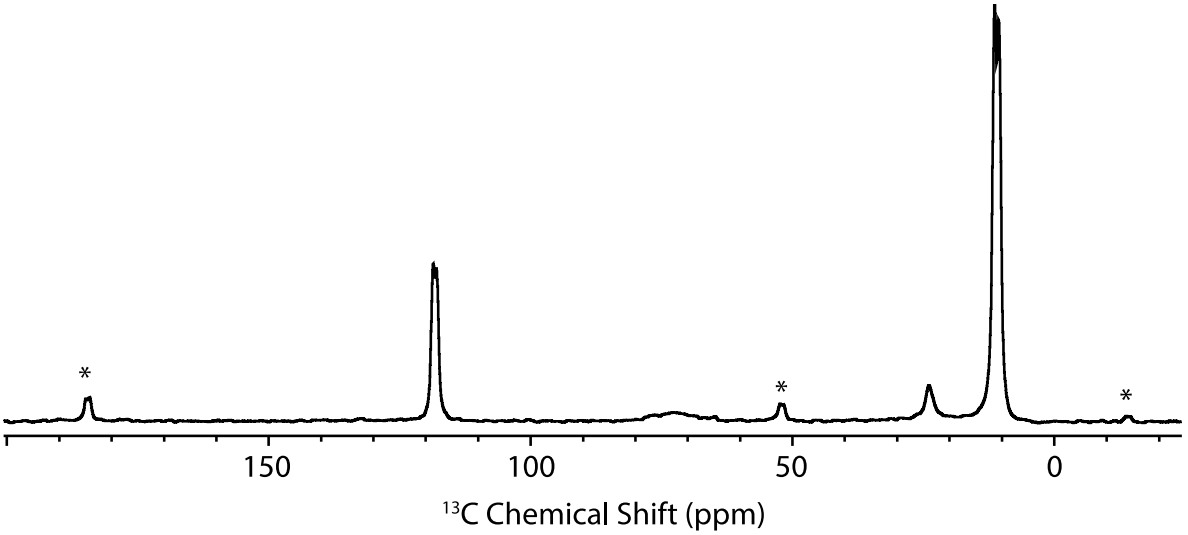
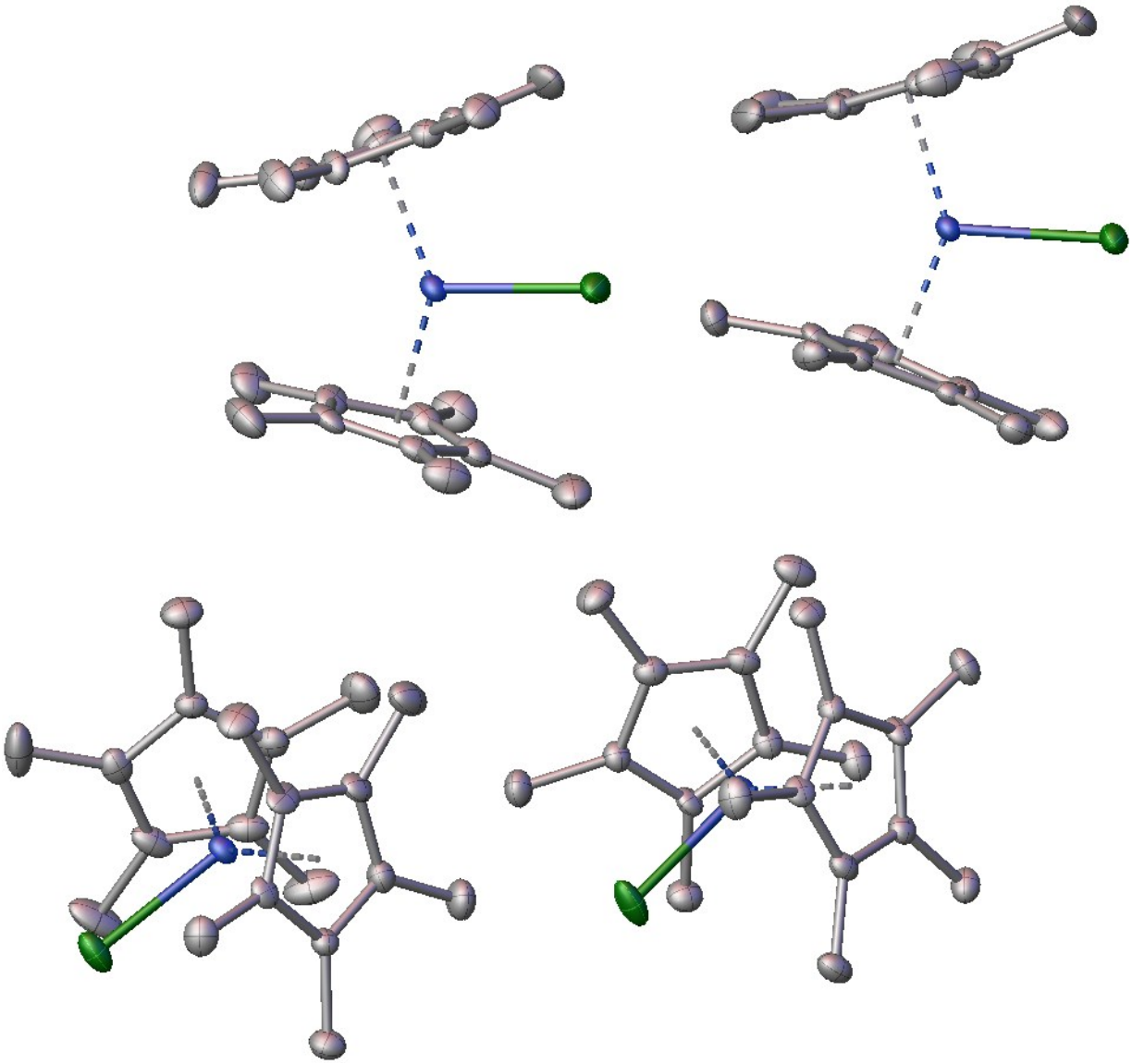


Figure S23. $^{13}C\{^{1}H\}$ CPMAS NMR spectrum of $Cp^*_2Sc–I$ at 10 kHz spinning speed (contact time = 2 ms; * = spinning sideband).



Cp*ScCl	Cp^*_a-Sc	Cp^*_b-Sc	Cp^*_a-Sc-Cp^*_b	Sc-Cl	Cp^*_a-Sc-Cl	Cp^*_b-Sc-Cl
Mol. 1	2.1471(128) Å	2.1572(127) Å	143.289(231)°	2.4183(15) Å	109.13	109.03.
Mol. 2	2.1514(78) Å	2.1650(146) Å	142.621(237)°	2.4079(16) Å	109.10	109.10
Mol. 3	2.1537(146) Å	2.1652(69) Å	142.992(254)°	2.4231(16) Å	107.75	109.60
Mol. 4	2.1545(106) Å	2.1622(117) Å	141.950(236)°	2.4206(16) Å	108.41	109.96
Average	2.1517(115) Å	2.1624(115) Å	142.713(240)°	2.4175(16) Å	108.57	109.44

Figure S24. Four independent molecules of Cp^*_2ScCl with 50% thermal ellipsoids with hydrogens omitted for clarity, bond distances for each molecule summarized in the table.

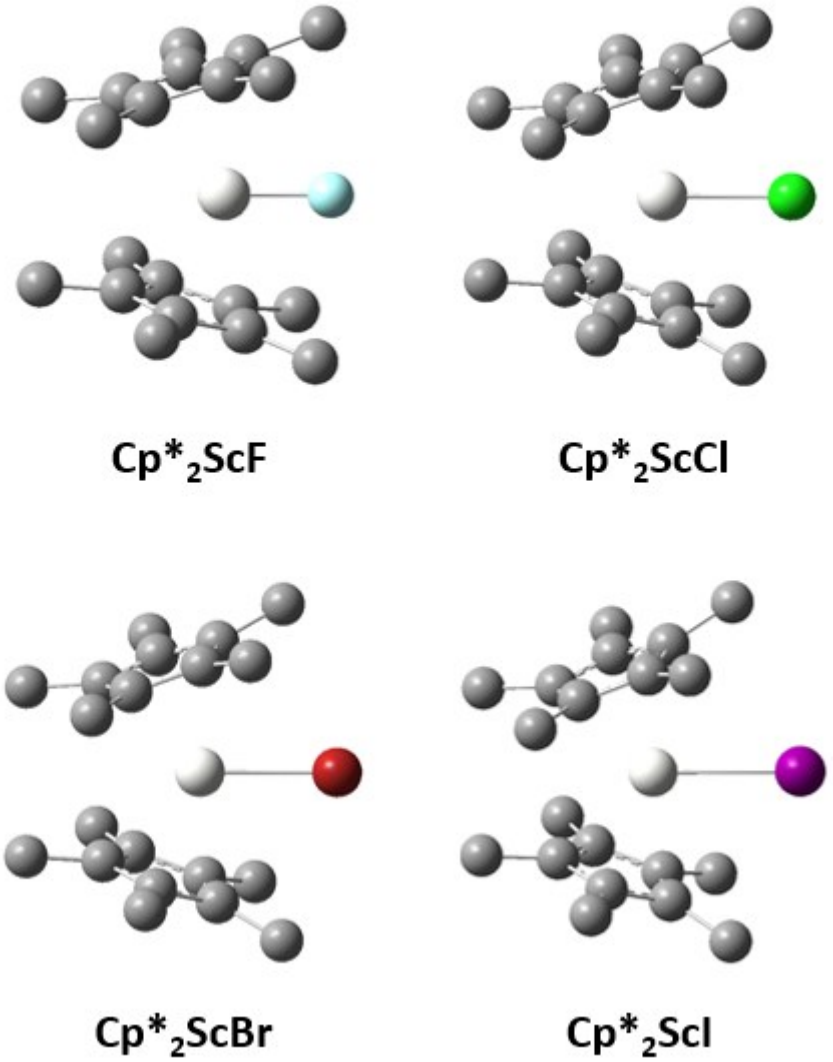


Figure S25. Geometry optimized structures of Cp*2Sc-X (X = F, Cl, Br, I) using B3LYP-GD3BJ, with SDD basis set for Sc, X and 6-31G(d,p) on C, H. Hydrogens omitted for clarity.

Table S4. Selected Geometry Optimized Parameters for Cp^*_2ScX (X = F, Cl, Br, I) from Figure S3.

	Cp^*_a-Sc	Cp^*_b-Sc	Cp^*_a-Sc-Cp^*_b	Sc-X	Cp^*_a-Sc-X	Cp^*_b-Sc-X
F	2.159 Å	2.159 Å	143.6°	1.917 Å	108.2°	108.2°
Cl	2.159 Å	2.159 Å	142.1°	2.435 Å	108.9°	108.9°
Br	2.161Å	2.162 Å	141.7°	2.604 Å	109.2°	109.1°
I	2.165 Å	2.166 Å	141.1°	2.840 Å	109.5°	109.5°

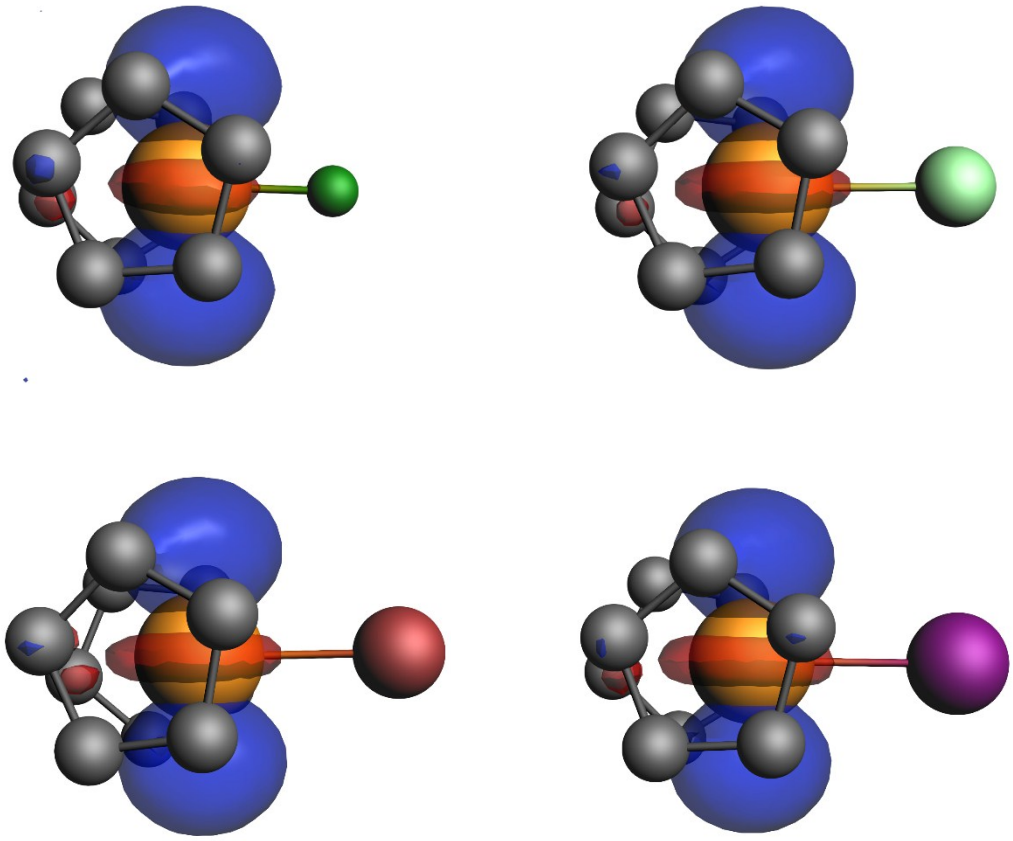


Figure S26. Kohn-Sham LUMOs for Cp^*_2ScX displaying a vacant $2a_1$ orbital for X = F (top left), Cl (top right), Br (bottom left), and I (bottom right). Top-down view, with isovalues of 0.04. Methyl groups omitted for clarity.

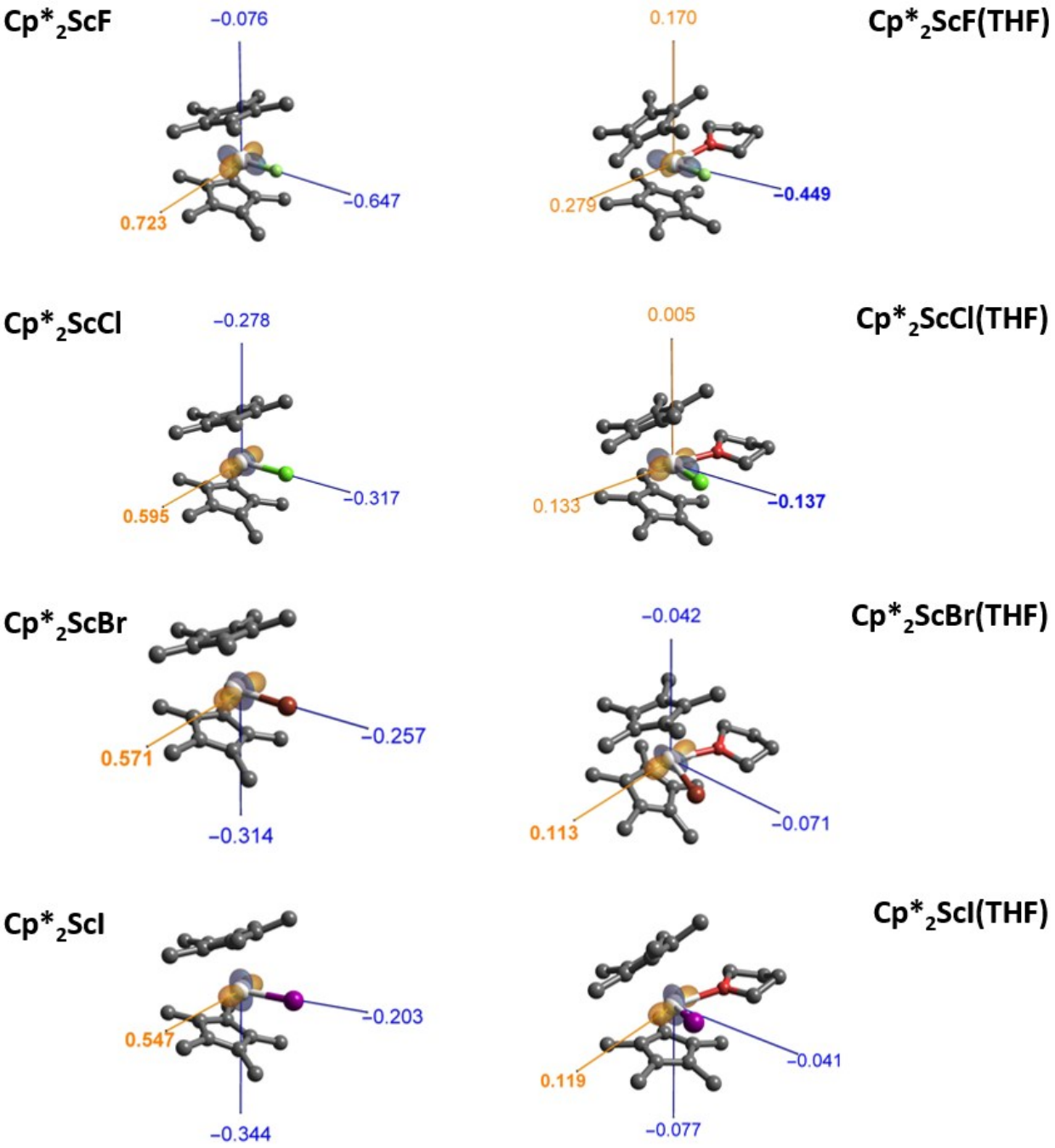


Figure S27. Calculated Electric Field Gradient Tensor Plots for Cp^*_2ScX and $Cp^*_2ScX(THF)$ for
X = F, Cl, Br, I. All hydrogens were omitted for clarity. Sc-Br and Sc-I bond lengths were manipulated for display purposes only.

Table S5. Summary of NLMO Contributions for V_{33} in Cp^*_2ScX in a.u.

X =	F	Cl	Br	I
Sc core	0.413	0.279	0.253	0.229
Cp*	0.009	0.068	0.021	0.021
X (core)	0.036	0.074	0.144	0.153
σ (Sc-X)	0.184	0.146	0.146	0.118
π_{b2}(Sc-X)	-0.022	-0.028	-0.029	-0.003
π_{b1}(Sc-X)	0.056	0.021	0.015	0.011
X (lone pair)	0.052	0.040	0.032	0.024
Total	0.728	0.600	0.583	0.553

Table S6. Summary of NLMO Contributions for V_{33} in $Cp^*_2ScX(THF)$ in a.u.

X =	F	Cl	Br	I
Sc core	-0.321	-0.048	-0.018	0.009
Cp*	0.379	0.312	0.328	0.388
X (core)	-0.081	-0.168	0.085	-0.003
σ (Sc-X)	-0.344	-0.224	0.074	0.025
π_{b2}(Sc-X)	-0.065	-0.024	0.011	0.005
$\pi 2a_1$(Sc-X)	-0.073	-0.030	-0.015	-0.016
X (lone pair)	-0.116	-0.072	0.019	0.004
THF_{core}	0.029	0.021	-0.075	-0.057
σ (Sc-O)	0.076	0.057	-0.136	-0.096
THF_{rest}	0.063	0.043	-0.173	-0.133
Total	-0.453	-0.133	0.100	0.126

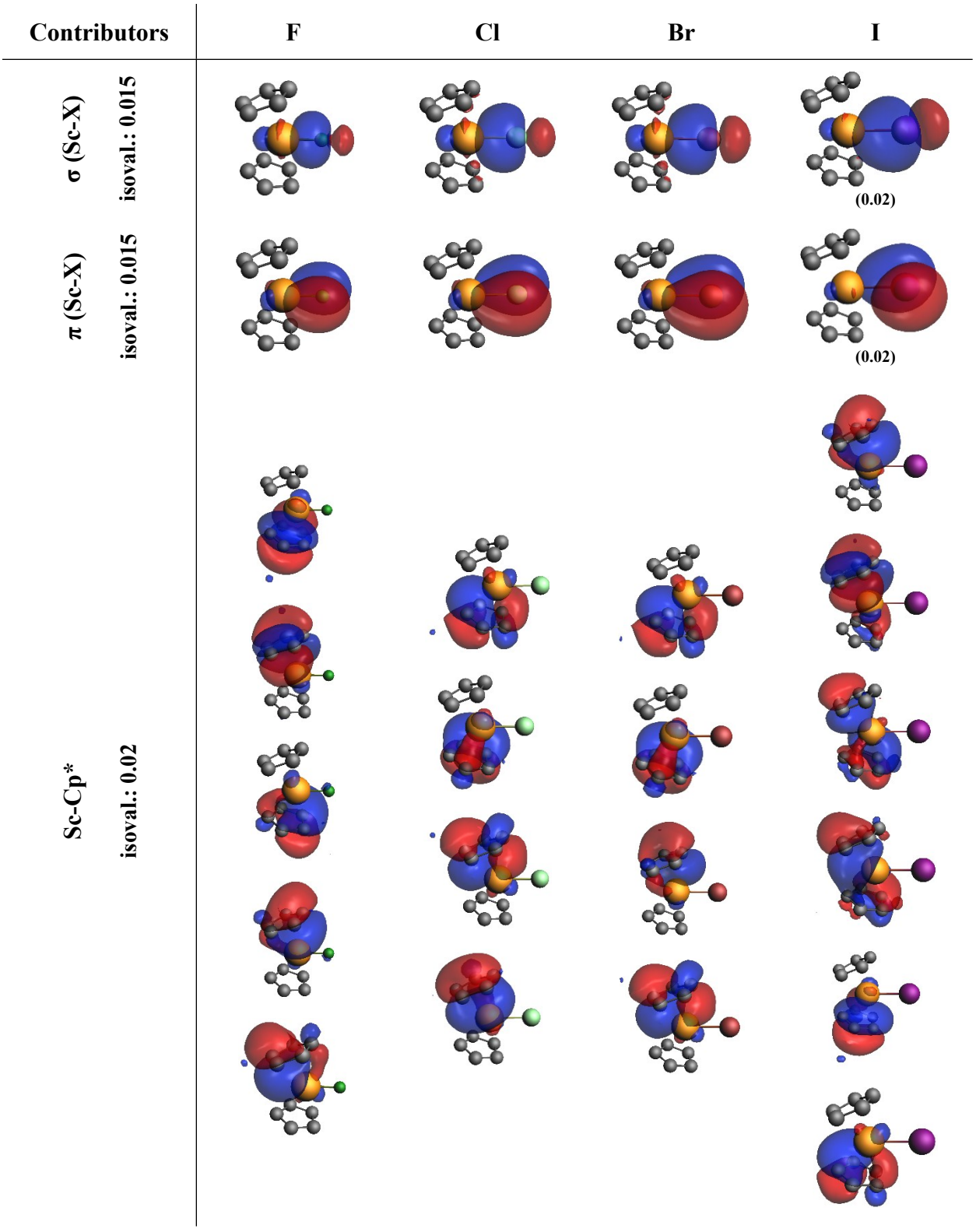


Figure S28. Selected NLMO Contributors for Cp^*_2ScX for X = F, Cl, Br, I. All methyl groups and hydrogens omitted for clarity. Values in parenthesis are altered isovalues, if applicable.

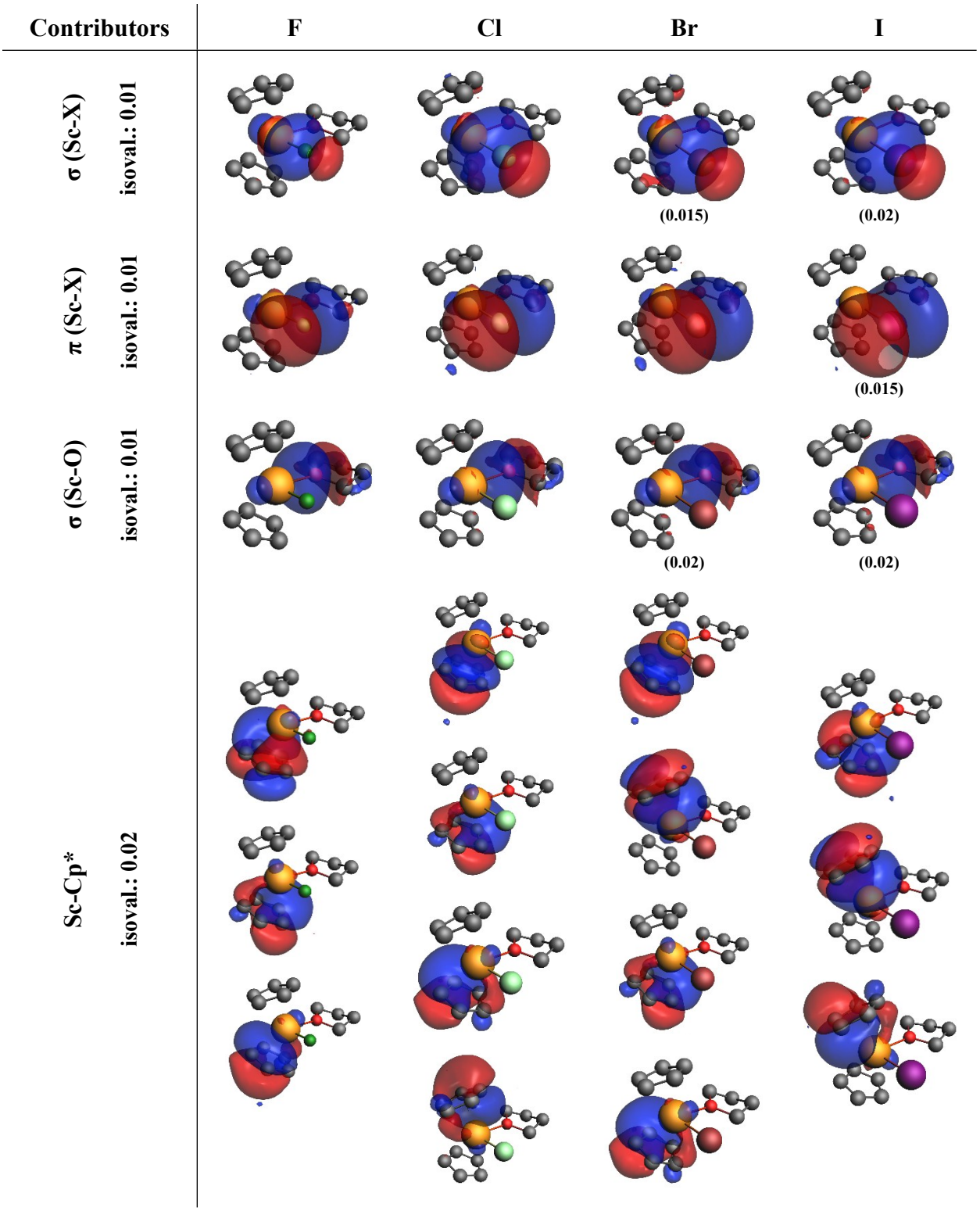


Figure S29. Selected NLMO Contributors for $Cp^*_2ScX(THF)$ for X = F, Cl, Br, I. All methyl groups and hydrogens omitted for clarity. Values in parentheses are altered isovalues, if applicable.

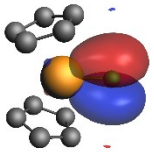
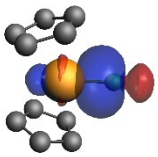
Contributions to V_{33}					
		σ (Sc-X)	**π_{b2} (Sc-X)**	**π_{b1} (Sc-X)**	**X (lone pair)**
X = F	**NLMO Contribution**	**0.184**	**-0.022**	**0.056**	**0.052**
	Ratio to Total	0.254	-0.030	0.077	0.072
X = Cl	**NLMO Contribution**	**0.146**	**-0.028**	**0.021**	**0.040**
	Ratio to Total	0.245	-0.047	0.035	0.067
X = Br	**NLMO Contribution**	**0.144**	**-0.029**	**0.015**	**0.032**
	Ratio to Total	0.252	-0.051	0.026	0.056
X = I	**NLMO Contribution**	**0.118**	**-0.003**	**0.011**	**0.024**
	Ratio to Total	0.216	-0.005	0.020	0.044

Figure S30. Selected NLMO Contributions from X in Cp^*_2ScX for X = F, Cl, Br, I. The NLMOs shown (isovalue = 0.015) are for X = F and are qualitative. All methyl groups and hydrogens omitted for clarity.

Full NLMO Decomposition Analysis for Cp^*_2ScX and $Cp^*_2ScX(THF)$ (X=F, Cl, Br, I):

All NLMO contributions to the principal component V_{33} are tabulated in the following pages. The default threshold for printing is 5%, but this setting did not print some halide lone pairs (both π-interactions and a lone pair) and misrepresented the Cp* contributions. Dropping the threshold for printing to 0% ensures that all contributions are described properly. Atomic contributions were rounded to nearest whole number. Rounding that resulted in 0% for scandium and less than 5% for all other atoms were not included in the following tables. The total calculated value and the total decomposed value after addition may vary because of error in rounding and subsequent addition. The analysis may assign halides to have four lone pairs in the valence orbitals, but plotting the orbitals unambiguously identifies σ(Sc-X) and π(Sc-X).

Table S7A. NLMO Contributions to V_{33} (in a.u.) for Cp^*_2ScF

NLMO no.	Orbital Type	Occ.	NLMO Composition	Lewis	non-Lewis	Total
1	core, Sc	2.00	100 Sc (100 1s)	-0.005	0.000	-0.005
2	core, Sc	2.00	100 Sc (100 2s)	-0.006	0.017	0.011
3	core, Sc	2.00	100 Sc (100 3s)	-0.032	-0.057	-0.089
4	core, Sc	2.00	100 Sc (100 2p)	176.477	-0.002	176.475
5	core, Sc	2.00	100 Sc (100 2p)	14.643	-0.111	14.532
6	core, Sc	2.00	100 Sc (100 2p)	177.906	-0.007	177.899
7	core, Sc	2.00	100 Sc (100 3p)	14.764	0.003	14.767
8	core, Sc	2.00	100 Sc (100 3p)	-354.409	0.050	-354.359
9	core, Sc	2.00	100 Sc (100 3p)	-28.895	0.077	-28.818
Sum of Sc core contributions:				**0.443**	**-0.030**	**0.413**
10	core, C2	2.00	100 C2 (100 1s)	0.007	0.000	0.007
11	core, C3	2.00	100 C3 (100 1s)	0.010	0.000	0.010
12	core, C4	2.00	100 C4 (100 1s)	-0.002	0.000	-0.002
13	core, C5	2.00	100 C5 (100 1s)	0.011	0.000	0.011
14	core, C6	2.00	100 C6 (100 1s)	0.004	0.000	0.004
15	core, C7	2.00	100 C7 (100 1s)	-0.006	0.000	-0.006
16	core, C8	2.00	100 C8 (100 1s)	-0.001	0.000	-0.001
17	core, C9	2.00	100 C9 (100 1s)	-0.012	0.000	-0.012
18	core, C10	2.00	100 C10 (100 1s)	-0.001	0.000	-0.001
19	core, C11	2.00	100 C11 (100 1s)	-0.008	0.000	-0.008
20	core, C12	2.00	100 C12 (100 1s)	0.010	0.000	0.010
21	core, C13	2.00	100 C13 (100 1s)	-0.002	0.000	-0.002
22	core, C14	2.00	100 C14 (100 1s)	0.012	0.000	0.012
23	core, C15	2.00	100 C15 (100 1s)	0.004	0.000	0.004
24	core, C16	2.00	100 C16 (100 1s)	0.007	0.000	0.007
25	core, C17	2.00	100 C17 (100 1s)	-0.002	0.000	-0.002
26	core, C18	2.00	100 C18 (100 1s)	-0.012	0.000	-0.012
27	core, C19	2.00	100 C19 (100 1s)	-0.001	0.000	-0.001
28	core, C20	2.00	100 C20 (100 1s)	-0.008	0.000	-0.008
29	core, C21	2.00	100 C21 (100 1s)	-0.006	0.000	-0.006
			Sum of Cp* core contributions:	**0.004**	**0.000**	**0.004**
31	lone pair, C4	1.12	49 C4 (0.8 2s, 99.2 2p) 11 Sc (0.6 4s, 0.2 4p, 99.2 3d) 10 C3 (0.3 2s, 99.7 2p) 9 C6 (0.6 2s, 99.4 2p) 9 C5 (0.9 2s, 99.1 2p) 9 C2 (0.2 2s, 99.8 2p)	-0.030	-0.111	-0.141
32	lone pair, C13	1.12	50 C13 (0.8 2s, 99.2 2p) 9 Sc (0.6 4s, 0.3 4p, 99.1 3d) 10 C15 (0.6 2s, 99.4 2p) 10 C13 (0.8 2s, 99.2 2p) 10 C12 (0.3 2s, 99.7 2p) 9 C14 (0.9 2s, 99.1 2p) 9 C16 (0.2 2s, 99.8 2p)	-0.034	-0.119	-0.153
37	bonding, C2-C3	1.95	49 C2 (29.6 2s, 70.4 2p) 49 C3 (29.5 2s, 70.5 2p) 1 Sc (7.3 4s, 5.5 4p, 87.3 3d)	0.014	0.001	0.015
38	bonding, C2-C3	1.68	43 C2 (0.4 2s, 99.6 2p) 40 C3 (0.4 3s, 99.7 2p) 7 Sc (2.8 4s, 0.3 4p, 96.9 3d)	0.030	0.086	0.116
39	bonding, C2-C6	1.95	49 C6 (29.4 2s, 70.5 2p) 49 C2 (29.9 2s, 70.2 2p) 1 Sc (7.6 4s, 9.0 4p, 83.4 3d)	0.003	0.001	0.004

40	bonding, C2-C7	1.98	50 C2 (30.1 2s, 69.9 2p) 49 C7 (28.7 2s, 71.3 2p)	-0.002	0.000	-0.002
41	bonding, C3-C4	1.95	49 C4 (29.7 2s, 70.3 2p) 49 C3 (29.8 2s, 70.2 2p) 1 Sc (6.7 4s, 8.7 4p, 84.6 3d)	0.003	0.001	0.004
42	bonding, C3-C8	1.98	51 C3 (30.2 2s, 69.8 2p) 49 C8 (28.5 2s, 71.5 2p)	0.003	0.000	0.003
43	bonding, C4-C5	1.94	49 C4 (29.3 2s, 70.8 2p) 49 C5 (28.9 2s, 71.1 2p) 1 Sc (6.8 4s, 11.7 4p, 81.6 3d)	0.006	0.001	0.007
44	bonding, C4-C9	1.98	50 C4 (29.8 2s, 70.2 2p) 49 C9 (28.9 2s, 71.1 2p)	-0.010	0.000	-0.010
45	bonding, C5-C6	1.95	49 C6 (29.5 2s, 70.6 2p) 49 C5 (29.4 2s, 70.6 2p) 1 Sc (6.1 4s, 11.4 4p, 82.5 3d)	0.011	0.001	0.012
46	bonding, C5-C6	1.70	42 C5 (1.0 2s, 99.0 2p) 42 C6 (0.8 2s, 99.2 2p) 6 Sc (4.7 4s, 1.0 4p, 94.3 3d)	0.028	0.067	0.095
47	bonding, C5-C10	1.98	50 C5 (30.0 2s, 70.0 2p) 49 C10 (28.8 2s, 71.3 2p)	0.004	0.000	0.004
48	bonding, C6-C11	1.98	50 C6 (30.0 2s, 70.0 2p) 49 C11 (28.8 2s, 71.2 2p)	-0.005	0.000	-0.005
49	bonding, C7-H22	1.98	62 C7 (22.6 2s, 77.4 2p) 37 H22 (100 1s)	-0.005	0.000	-0.005
50	bonding, C7-H23	1.98	61 C7 (22.1 2s, 77.9 2p) 38 H23 (100 1s)	-0.010	0.000	-0.010
51	bonding, C7-H24	1.97	61 C7 (22.1 2s, 77.9 2p) 37 H24 (100 1s)	-0.005	0.000	-0.005
52	bonding, C8-H25	1.97	61 C8 (22.1 2s, 77.9 2p) 38 H25 (100 1s)	-0.003	0.001	-0.002
53	bonding, C8-H26	1.98	61 C8 (22.0 2s, 78.0 2p) 38 H26 (100 1s)	-0.005	0.000	-0.005
54	bonding, C8-H27	1.98	62 C8 (22.8 2s, 77.2 2p) 37 H27 (100 1s)	0.000	0.001	0.001
55	bonding, C9-H28	1.98	61 C9 (22.4 2s, 77.6 2p) 38 H28 (100 1s)	-0.013	0.000	-0.013
56	bonding, C9-H29	1.98	61 C9 (22.2 2s, 77.8 2p) 38 H29 (100 1s)	-0.014	0.000	-0.014
57	bonding, C9-H30	1.97	61 C9 (22.0 2s, 78.0 2p) 37 H30 (100 1s)	-0.008	-0.003	-0.011
58	bonding, C10-H31	1.97	61 C10 (22.0 2s, 78.0 2p) 37 H31 (100 1s)	-0.002	0.002	0.000
59	bonding, C10-H32	1.98	61 C10 (22.4 2s, 77.6 2p) 38 H32 (100 1s)	-0.001	0.000	-0.001
60	bonding, C10-H33	1.98	61 C10 (22.1 2s, 77.9 2p) 38 H33 (100 1s)	-0.002	0.000	-0.002
61	bonding, C11-H34	1.97	61 C11 (22.1 2s, 77.9 2p) 37 H34 (100 1s)	-0.006	-0.001	-0.007
62	bonding, C11-H35	1.98	61 C11 (22.1 2s, 77.9 2p) 38 H35 (100 1s)	-0.012	0.000	-0.012
63	bonding, C11-H36	1.98	61 C11 (22.3 2s, 77.7 2p) 38 H36 (100 1s)	-0.007	0.000	-0.007
64	bonding, C12-C13	1.95	49 C12 (29.9 2s, 70.1 2p) 49 C13 (29.7 2s, 70.3 2p) 1 Sc (6.8 4s, 8.6 4p, 84.6 3d)	0.003	0.001	0.004
65	bonding, C12-C16	1.95	49 C16 (29.6 2s, 70.4 2p) 49 C12 (29.4 2s, 70.6 2p) 1 Sc (7.2 4s, 5.5 4p, 87.2 3d)	0.014	0.001	0.015
66	bonding, C12-C16	1.68	43 C16 (0.4 2s, 99.6 2p) 40 C12 (0.4 2s, 99.6 2p) 6 Sc (2.6 4s, 0.3 4p, 97.0 3d)	0.032	0.084	0.116
67	bonding, C12-C17	1.98	51 C12 (30.3 2s, 69.7 2p) 49 C17 (28.5 2s, 71.5 2p)	0.003	0.000	0.003
68	bonding, C13-C14	1.94	49 C13 (29.2 2s, 70.8 2p) 49 C14 (28.8 2s, 71.2 2p) 1 Sc (6.8 4s, 11.7 4p, 81.5 3d)	0.006	0.001	0.007
69	bonding, C13-C18	1.98	50 C13 (29.9 2s, 70.1 2p) 49 C18 (29.0 2s, 71.0 2p)	-0.010	0.000	-0.010
70	bonding, C14-C15	1.95	49 C15 (29.4 2s, 70.6 2p) 49 C14 (29.4 2s, 70.6 2p) 1 Sc (6.3 4s, 11.5 4p, 82.2 3d)	0.011	0.001	0.012
71	bonding, C14-C15	1.70	42 C14 (1.0 2s, 99.0 2p) 42 C15 (0.8 2s, 99.2 2p) 7 Sc (3.8 4s, 1.0 4p, 95.2 3d)	0.025	0.069	0.094
72	bonding, C14-C19	1.98	50 C14 (30.0 2s, 70.0 2p) 49 C19 (28.8 2s, 71.3 2p)	0.004	0.000	0.004
73	bonding, C15-C16	1.95	49 C15 (29.4 2s, 70.6 2p) 49 C16 (29.9 2s, 70.1 2p) 1 Sc (7.6 4s, 8.9 4p, 83.5 3d)	0.003	0.001	0.004
74	bonding, C15-C20	1.98	50 C15 (30.0 2s, 70.0 2p) 49 C20 (28.9 2s, 71.1 2p)	-0.005	0.000	-0.005

75	bonding, C16-C21	1.98	50 C16 (30.1 2s, 69.9 2p) 49 C21 (28.6 2s, 71.4 2p)	-0.002	0.000	-0.002
76	bonding, C17-H37	1.98	62 C17 (22.7 2s, 77.3 2p) 37 H37 (100 1s)	0.000	0.001	0.001
77	bonding, C17-H38	1.97	61 C17 (22.1 2s, 77.9 2p) 38 H38 (100 1s)	-0.003	0.001	-0.002
78	bonding, C17-H39	1.98	61 C17 (22.1 2s, 77.9 2p) 38 H39 (100 1s)	-0.005	0.000	-0.005
79	bonding, C18-H40	1.98	61 C18 (22.1 2s, 77.9 2p) 38 H40 (100 1s)	-0.014	0.000	-0.014
80	bonding, C18-H41	1.97	61 C18 (22.1 2s, 77.9 2p) 37 H41 (100 1s)	-0.008	-0.003	-0.011
81	bonding, C18-H42	1.98	61 C18 (22.4 2s, 77.7 2p) 38 H42 (100 1s)	-0.013	0.000	-0.013
82	bonding, C19-H43	1.98	61 C19 (22.4 2s, 77.6 2p) 38 H43 (100 1s)	-0.001	0.000	-0.001
83	bonding, C19-H44	1.98	61 C19 (22.1 2s, 77.9 2p) 38 H44 (100 1s)	-0.002	0.000	-0.002
84	bonding, C19-H45	1.97	61 C19 (21.9 2s, 78.1 2p) 37 H45 (100 1s)	-0.002	0.002	0.000
85	bonding, C20-H46	1.97	61 C20 (22.1 2s, 77.9 2p) 37 H46 (100 1s)	-0.006	-0.001	-0.007
86	bonding, C20-H47	1.98	61 C20 (22.1 2s, 77.9 2p) 38 H47 (100 1s)	-0.012	0.000	-0.012
87	bonding, C20-H48	1.98	61 C20 (22.3 2s, 77.7 2p) 38 H48 (100 1s)	-0.007	0.000	-0.007
88	bonding, C21-H49	1.97	61 C21 (22.1 2s, 77.9 2p) 37 H49 (100 1s)	-0.005	0.000	-0.005
89	bonding, C21-H50	1.98	62 C21 (22.6 2s, 77.4 2p) 37 H50 (100 1s)	-0.005	0.000	-0.005
90	bonding, C21-H51	1.98	61 C21 (22.1 2s, 77.9 2p) 38 H51 (100 1s)	-0.010	0.000	-0.010
			Sum of Cp* lone pair / bonding orbital contributions:	**-0.081**	**0.086**	**0.005**
30	core, F	2.00	100 F (100 2s)	0.036	0.000	0.036
			Sum of F core contributions:	**0.036**	**0.000**	**0.036**
33	lone pair, F	1.95	98 F (45.7 2s, 54.3 2p) 2 Sc (17.3 4s, 0.3 4p, 82.4 3d)	0.041	0.011	0.052
34	lone pair, F	1.93	96 F (100 2p) 3 Sc (0.6 4p, 99.4 3d)	0.030	0.026	0.056
35	lone pair, F	1.89	94 F (100 2p) 6 Sc (0.8 4p, 99.2 3d)	0.015	-0.037	-0.022
36	lone pair, F	1.88	93 F52 (54.3 2s, 45.7 2p) 6 Sc (5.4 4s, 0.1 4p, 94.4 3d)	0.120	0.064	0.184
			Sum of F lone pair / bonding contributions:	**0.206**	**0.064**	**0.270**
			Total (0.723 calc'd):	**0.608**	**0.120**	**0.728**

Table S7B. NLMO Contributions to V_{33} (in a.u.) for Cp^*_2ScCl

NLMO no.	Orbital Type	Occ.	NLMO Composition	Lewis	non-Lewis	Total
1	core, Sc	2.00	100 Sc (100 1s)	-0.005	0.001	-0.004
2	core, Sc	2.00	100 Sc (100 2s)	-0.007	0.014	0.007
3	core, Sc	2.00	100 Sc (100 3s)	-0.024	-0.056	-0.080
4	core, Sc	2.00	100 Sc (100 2p)	176.448	0.000	176.448
5	core, Sc	2.00	100 Sc (100 2p)	14.163	-0.106	14.057
6	core, Sc	2.00	100 Sc (100 2p)	178.348	-0.012	178.336
7	core, Sc	2.00	100 Sc (100 3p)	14.199	-0.009	14.190
8	core, Sc	2.00	100 Sc (100 3p)	-354.820	0.049	-354.771
9	core, Sc	2.00	100 Sc (100 3p)	-27.970	0.066	-27.904
			Sum of Sc core contributions:	**0.332**	**-0.053**	**0.279**
15	core, C3	2.00	100 C3 (100 1s)	0.007	0.000	0.007
16	core, C4	2.00	100 C4 (100 1s)	0.010	0.000	0.010
17	core, C5	2.00	100 C5 (100 1s)	-0.002	0.000	-0.002
18	core, C6	2.00	100 C6 (100 1s)	0.012	0.000	0.012
19	core, C7	2.00	100 C7 (100 1s)	0.004	0.000	0.004
20	core, C8	2.00	100 C8 (100 1s)	-0.005	0.000	-0.005
21	core, C9	2.00	100 C9 (100 1s)	-0.002	0.000	-0.002
22	core, C10	2.00	100 C10 (100 1s)	-0.012	0.000	-0.012
23	core, C11	2.00	100 C11 (100 1s)	0.000	0.000	0.000
24	core, C12	2.00	100 C12 (100 1s)	-0.008	0.000	-0.008
25	core, C13	2.00	100 C13 (100 1s)	0.010	0.000	0.010
26	core, C14	2.00	100 C14 (100 1s)	-0.002	0.000	-0.002
27	core, C15	2.00	100 C15 (100 1s)	0.012	0.000	0.012
28	core, C16	2.00	100 C16 (100 1s)	0.004	0.000	0.004
29	core, C17	2.00	100 C17 (100 1s)	0.007	0.000	0.007
30	core, C18	2.00	100 C18 (100 1s)	-0.002	0.000	-0.002
31	core, C19	2.00	100 C19 (100 1s)	-0.012	0.000	-0.012
32	core, C20	2.00	100 C20 (100 1s)	0.000	0.000	0.000
33	core, C21	2.00	100 C21 (100 1s)	-0.008	0.000	-0.008
34	core, C22	2.00	100 C22 (100 1s)	-0.005	0.000	-0.005
			Sum of Cp* core contributions:	**0.008**	**0.000**	**0.008**
37	lone pair, C5	1.11	42 C5 (1.1 2s, 98.8 2p) 40 C4 (0.8 2s, 99.2 2p) 7 Sc (5.2 4s, 0.5 4p, 94.3 3d)	-0.016	-0.002	-0.018
38	lone pair, C6	1.09	48 C6 (1.5 2s, 98.5 2p) 11 C7 (1.4 2s, 98.7 2p) 10 Sc (0.8 4s, 0.3 4p, 98.9 3d) 10 C4 (0.5 2s, 99.5 2p) 9 C3 (0.5 2s, 99.5 2p) 9 C5 (1.3 2s, 98.7 2p)	0.015	0.135	0.150
39	lone pair, C7	1.11	41 C7 (1.3 2s, 98.7 2p) 40 C3 (0.9 2s, 99.1 2p) 8 Sc (3.0 4s, 0.4 4p, 96.6 3d)	-0.009	-0.046	-0.055
40	lone pair, C14	1.11	42 C14 (1.1 2s, 98.9 2p) 40 C13 (0.8 2s, 99.2 2p) 7 Sc (5.5 4s, 0.4 4p, 94.1 3d)	-0.015	0.001	-0.014
41	lone pair, C15	1.11	48 C15 (1.5 2s, 98.5 2p) 11 C16 (1.4 2s, 98.7 2p) 11 Sc (0.8 4s, 0.3 4p, 98.9 3d) 10 C13 (0.5 2s, 99.5 2p) 9 C14 (1.3 2s, 98.7 2p)	0.015	0.135	0.150
42	lone pair, C16	1.09	42 C16 (1.3 2s, 98.7 2p) 40 C17 (0.9 2s, 99.1 2p) 8 Sc (3.0 4s, 0.4 4p, 96.6 3d)	-0.009	-0.046	-0.055

45	bonding, C3-C4	1.95	49 C3 (29.6 2s, 70.6 2p) 49 C4(29.5 2s, 70.5 2p)	0.014	0.001	0.015
46	bonding, C3-C7	1.95	49 C7 (28.8 2s, 71.2 2p) 49 C3 (29.0 2s, 71.0 2p) 1 Sc (6.4 4s, 11.9 4p, 81.7 3d)	0.003	0.001	0.004
47	bonding, C3-C8	1.98	51 C3 (30.2 2s, 69.8 2p) 49 C8 (28.5 2s, 71.5 2p)	-0.001	0.000	-0.001
48	bonding, C4-C5	1.95	49 C5 (29.4 2s, 70.7 2p) 49 C4 (28.9 2s, 71.1 2p) 1 Sc (5.1 4s, 9.9 4p, 85.0 3d)	0.003	0.001	0.004
49	bonding, C4-C9	1.98	51 C4 (30.4 2s, 69.6 2p) 48 C9 (28.5 2s, 71.5 2p)	0.003	0.000	0.003
50	bonding, C5-C6	1.94	49 C5 (29.1 2s, 70.9 2p) 49 C6 (28.4 2s, 71.6 2p) 1 Sc (5.1 4s, 13.1 4p, 81.8 3d)	0.006	0.001	0.007
51	bonding, C5-C10	1.98	50 C5 (29.7 2s, 70.3 2p) 49 C10 (28.9 2s, 71.1 2p)	-0.010	0.000	-0.010
52	bonding, C6-C7	1.95	49 C7 (29.3 2s, 70.8 2p) 49 C6 (29.1 2s, 70.9 2p) 1 Sc (4.1 4s, 11.3 4p, 84.6 3d)	0.012	0.001	0.013
53	bonding, C6-C11	1.98	50 C6 (29.9 2s, 70.1 2p) 49 C11 (28.6 2s, 71.4 2p)	0.005	0.000	0.005
54	bonding, C7-C12	1.98	50 C7 (29.9 2s, 70.1 2p) 49 C12 (28.8 2s, 71.2 2p)	-0.004	0.000	-0.004
55	bonding, C8-H23	1.98	62 C8 (22.9 2s, 77.1 2p) 37 H23 (100 1s)	-0.004	0.000	-0.004
56	bonding, C8-H24	1.98	61 C8 (22.0 2s, 78.0 2p) 38 H24 (100 1s)	-0.009	0.000	-0.009
57	bonding, C8-H25	1.97	61 C8 (22.0 2s, 78.0 2p) 37 H25 (100 1s)	-0.004	0.000	-0.004
58	bonding, C9-H26	1.97	61 C9 (22.0 2s, 78.0 2p) 38 H26 (100 1s)	-0.002	0.002	0.000
59	bonding, C9-H27	1.98	61 C9 (22.1 2s, 77.9 2p) 38 H27 (100 1s)	-0.005	0.000	-0.005
60	bonding, C9-H28	1.98	62 C9 (22.9 2s, 77.1 2p) 37 H28 (100 1s)	0.000	0.000	0.000
61	bonding, C10-H29	1.98	61 C10 (22.4 2s, 77.6 2p) 38 H29 (100 1s)	-0.012	0.000	-0.012
62	bonding, C10-H30	1.98	61 C10 (22.2 2s, 77.8 2p) 38 H30 (100 1s)	-0.013	0.000	-0.013
63	bonding, C10-H31	1.97	61 C10 (22.1 2s, 78.0 2p) 37 H31 (100 1s)	-0.008	-0.002	-0.010
64	bonding, C11-H32	1.97	61 C11 (21.9 2s, 78.2 2p) 37 H32 (100 1s)	-0.001	0.002	0.001
65	bonding, C11-H33	1.98	61 C11 (22.5 2s, 77.6 2p) 38 H33 (100 1s)	-0.001	0.000	-0.001
66	bonding, C11-H34	1.98	61 C11 (22.2 2s, 77.8 2p) 38 H34 (100 1s)	-0.002	0.000	-0.002
67	bonding, C12-H35	1.97	61 C12 (22.1 2s, 77.9 2p) 37 H35 (100 1s)	-0.006	-0.001	-0.007
68	bonding, C12-H36	1.98	61 C12 (22.2 2s, 77.8 2p) 38 H36 (100 1s)	-0.012	0.000	-0.012
69	bonding, C12-H37	1.98	61 C12 (22.3 2s, 77.7 2p) 38 H37 (100 1s)	-0.007	0.000	-0.007
70	bonding, C13-C14	1.95	49 C14 (29.3 2s, 70.7 2p) 49 C13 (28.9 2s, 71.1 2p) 1 Sc (5.1 4s, 9.8 4p, 85.1 3d)	0.003	0.001	0.004
71	bonding, C13-C17	1.95	49 C17 (29.6 2s, 70.4 2p) 49 C13 (29.4 2s, 70.6 2p)	0.014	0.001	0.015
72	bonding, C13-C18	1.98	51 C13 (30.4 2s, 69.6 2p) 48 C18 (28.5 2s, 71.5 2p)	0.003	0.000	0.003
73	bonding, C14-C15	1.94	49 C14 (29.1 2s, 70.9 2p) 49 C15 (28.4 2s, 71.6 2p) 1 Sc (5.0 4s, 13.1 4p, 81.9 3d)	0.006	0.001	0.007
74	bonding, C14-C19	1.98	50 C14 (29.7 2s, 70.3 2p) 49 C19 (28.9 2s, 71.1 2p)	-0.010	0.000	-0.010
75	bonding , C15-C16	1.95	49 C16 (29.3 2s, 70.7 2p) 49 C15 (29.2 2s, 70.9 2p) 1 Sc (4.0 4s, 11.3 4p, 84.7 3d)	0.012	0.001	0.013
76	bonding, C15-C20	1.98	50 C15 (29.9 2s, 70.1 2p) 49 C20 (28.6 2s, 71.4 2p)	0.005	0.000	0.005
77	bonding, C16-C17	1.95	49 C16 (28.8 2s, 71.2 2p) 49 C17 (29.0 2s, 71.0 2p) 1 Sc (6.4 4s, 11.7 4p, 81.9 3d)	0.003	0.001	0.004
78	bonding, C16-C21	1.98	50 C16 (30.0 2s, 70.1 2p) 49 C21 (28.8 2s, 71.2 2p)	-0.004	0.000	-0.004
79	bonding, C17-C22	1.98	51 C17 (30.2 2s, 69.8 2p) 49 C22 (28.6 2s, 71.4 2p)	-0.001	0.000	-0.001

80	bonding, C18-H38	1.98	62 C18 (22.9 2s, 77.2 2p) 37 H38 (100 1s)	0.000	0.000	0.000
81	bonding, C18-H39	1.97	61 C18 (22.0 2s, 78.0 2p) 38 H39 (100 1s)	-0.002	0.002	0.000
82	bonding, C18-H40	1.98	61 C18 (22.1 2s, 77.9 2p) 38 H40 (100 1s)	-0.005	0.000	-0.005
83	bonding, C19-H41	1.98	61 C19 (22.2 2s, 77.8 2p) 38 H41 (100 1s)	-0.013	0.000	-0.013
84	bonding, C19-H42	1.97	61C19 (22.0 2s, 78.0 2p) 37 H42 (100 1s)	-0.008	-0.002	-0.010
85	bonding, C19-H43	1.98	61 C19 (22.4 2s, 77.7 2p) 38 H43 (100 1s)	-0.012	0.000	-0.012
86	bonding, C20-H44	1.98	61 C20 (22.4 2s, 77.6 2p) 38 H44 (100 1s)	-0.001	0.000	-0.001
87	bonding, C20-H45	1.98	61 C20 (22.2 2s, 77.8 2p) 38 H45 (100 1s)	-0.002	0.000	-0.002
88	bonding, C20-H46	1.97	61 C20 (21.9 2s, 78.1 2p) 37 H46 (100 1s)	-0.001	0.002	0.001
89	bonding, C21-H47	1.97	61 C21 (22.1 2s, 77.9 2p) 37 H47 (100 1s)	-0.006	-0.001	-0.007
90	bonding, C21-H48	1.98	61 C21 (22.1 2s, 77.9 2p) 38 H48 (100 1s)	-0.012	0.000	-0.012
91	bonding, C21-H49	1.98	61 C21 (22.3 2s, 77.7 2p) 38 H49 (100 1s)	-0.007	0.000	-0.007
92	bonding, C22-H50	1.97	61 C22 (22.1 2s, 78.0 2p) 37 H50 (100 1s)	-0.004	0.000	-0.004
93	bonding, C22-H51	1.98	62 C22 (22.8 2s, 77.2 2p) 37 H51 (100 1s)	-0.004	0.000	-0.004
94	bonding, C22-H52	1.98	61 C22 (22.0 2s, 78.0 2p) 38 H52 (100 1s)	-0.009	0.000	-0.009
			Sum of Cp* lone pair / bonding orbital contributions:	**-0.129**	**0.189**	**0.060**
10	core, Cl	2.00	100 Cl (100 1s)	0.015	0.000	0.015
11	core, Cl	2.00	100 Cl (100 2s)	0.015	0.000	0.015
12	core, Cl	2.00	100 Cl (100 2p)	0.015	0.000	0.015
13	core, Cl	2.00	100 Cl (100 2p)	0.015	0.000	0.015
14	core, Cl	2.00	100 Cl (100 2p)	0.014	0.000	0.014
			Sum of Cl core contributions:	**0.074**	**0.000**	**0.074**
35	lone pair, Cl	1.97	98 Cl (52.8 2s, 47.2 2p) 1 Sc (11.4 4s, 0.9 4p, 87.7 3d)	0.028	0.012	0.040
36	lone pair, Cl	1.92	96 Cl (100 2p) 3 Sc (0.7 4p, 99.3 3d)	0.006	0.015	0.021
43	lone pair, Cl	1.99	87 Cl (47.3 2s, 52.7 2p) 12 Sc (15.1 4s, 0.5 4p, 84.4 3d)	0.141	0.005	0.146
44	lone pair, Cl	1.99	92 Cl (100 2p) 7 Sc (0.8 4p, 99.2 3d)	-0.026	-0.002	-0.028
			Sum of Cl lone pair / bonding contributions:	**0.149**	**0.030**	**0.179**
			Total (0.595 calc'd):	**0.434**	**0.166**	**0.600**

Table S7C. NLMO Contributions to V_{33} (in a.u.) for Cp^*_2ScBr

NLMO no.	Orbital Type	Occ.	NLMO Composition	Lewis	non-Lewis	Total
1	core, Sc	2.00	100 Sc (100 1s)	-0.005	0.001	-0.004
2	core, Sc	2.00	100 Sc (100 2s)	-0.007	0.012	0.005
3	core, Sc	2.00	100 Sc (100 3s)	-0.024	-0.053	-0.077
4	core, Sc	2.00	100 Sc (100 2p)	178.449	0.001	178.450
5	core, Sc	2.00	100 Sc (100 2p)	14.231	-0.108	14.123
6	core, Sc	2.00	100 Sc (100 2p)	180.229	-0.009	180.220
7	core, Sc	2.00	100 Sc (100 3p)	14.232	-0.009	14.223
8	core, Sc	2.00	100 Sc (100 3p)	-358.695	0.041	-358.654
9	core, Sc	2.00	100 Sc (100 3p)	-28.098	0.065	-28.033
			Sum of Sc core contributions:	**0.312**	**-0.059**	**0.253**
10	core, C2	2.00	100 C2 (100 1s)	0.007	0.000	0.007
11	core, C3	2.00	100 C3 (100 1s)	0.010	0.000	0.010
12	core, C4	2.00	100 C4 (100 1s)	-0.002	0.000	-0.002
13	core, C5	2.00	100 C5 (100 1s)	0.012	0.000	0.012
14	core, C6	2.00	100 C6 (100 1s)	0.004	0.000	0.004
15	core, C7	2.00	100 C7 (100 1s)	-0.006	0.000	-0.006
16	core, C8	2.00	100 C8 (100 1s)	-0.002	0.000	-0.002
17	core, C9	2.00	100 C9 (100 1s)	-0.012	0.000	-0.012
18	core, C10	2.00	100 C10 (100 1s)	-0.001	0.000	-0.001
19	core, C11	2.00	100 C11 (100 1s)	-0.009	0.000	-0.009
20	core, C12	2.00	100 C12 (100 1s)	0.010	0.000	0.010
21	core, C13	2.00	100 C13 (100 1s)	-0.002	0.000	-0.002
22	core, C14	2.00	100 C14 (100 1s)	0.012	0.000	0.012
23	core, C15	2.00	100 C15 (100 1s)	0.004	0.000	0.004
24	core, C16	2.00	100 C16 (100 1s)	0.007	0.000	0.007
25	core, C17	2.00	100 C17 (100 1s)	-0.002	0.000	-0.002
26	core, C18	2.00	100 C18 (100 1s)	-0.012	0.000	-0.012
27	core, C19	2.00	100 C19 (100 1s)	-0.001	0.000	-0.001
28	core, C20	2.00	100 C20 (100 1s)	-0.008	0.000	-0.008
29	core, C21	2.00	100 C21 (100 1s)	-0.006	0.000	-0.006
			Sum of Cp* core contributions:	**0.003**	**0.000**	**0.003**
44	lone pair, C4	1.11	42 C4 (1.1 2s, 98.9 2p) 40 C3 (0.8 2s, 99.2 2p) 7 Sc (5.6 4s, 0.4 4p, 93.9 3d)	-0.015	0.000	-0.015
45	lone pair, C5	1.09	47 C5 (1.5 2s, 98.5 2p) 11 Sc (0.7 4s, 0.3 4p, 99.1 3d) 11 C6 (1.3 2s, 98.7 2p) 10 C3 (0.5 2s, 99.5 2p) 9 C2 (0.6 2s, 99.5 2p) 9 C4 (1.3 2s, 98.7 2p)	0.013	0.135	0.148
46	lone pair, C6	1.11	42 C6 (1.3 2s, 98.7 2p) 40 C2 (0.9 2s, 99.1 2p) 8 Sc (3.1 4s, 0.4 4p, 96.4 3d)	-0.009	-0.047	-0.056
47	lone pair, C13	1.11	42 C13 (1.1 2s, 98.9 2p) 40 C12 (0.8 2s, 99.2 2p) 6 Sc (5.4 4s, 0.6 4p, 94.0 3d)	-0.016	-0.001	-0.017
48	lone pair, C14	1.09	48 C14 (1.5 2s, 98.6 2p) 11 C15 (1.3 2s, 98.7 2p) 10 Sc (1.0 4s, 0.3 4p, 98.7 3d) 10 C12 (0.5 2s, 99.5 2p) 9 C13 (1.3 2s, 98.7 2p)	0.016	0.131	0.147
49	lone pair, C15	1.11	42 C15 (1.3 2s, 98.7 2p) 40 C16 (0.9 2s, 99.1 2p) 8 Sc (3.1 4s, 0.5 4p, 96.4 3d)	-0.009	-0.048	-0.057

54	bonding, C2-C3	1.95	49 C2 (29.7 2s, 70.3 2p) 49 C3 (29.7 2s, 70.4 2p)	0.013	0.001	0.014
55	bonding, C2-C6	1.95	49 C6 (28.8 2s, 71.2 2p) 49 C2 (29.0 2s, 71.0 2p) 1 Sc (6.4 4s, 11.4 4p, 82.2 3d)	0.003	0.001	0.004
56	bonding, C2-C7	1.98	51 C2 (30.2 2s, 69.8 2p) 49 C7 (28.6 2s, 71.4 2p)	-0.002	0.000	-0.002
57	bonding, C3-C4	1.95	49 C4 (29.3 2s, 70.7 2p) 49 C3 (28.8 2s, 71.3 2p) 1 Sc (5.2 4s, 9.7 4p, 85.1 3d)	0.003	0.001	0.004
58	bonding, C3-C8	1.98	51 C3 (30.4 2s, 69.6 2p) 48 C8 (28.4 2s, 71.6 2p)	0.002	0.000	0.002
59	bonding, C4-C5	1.94	49 C4 (29.2 2s, 70.8 2p) 49 C5 (28.5 2s, 71.5 2p) 1 Sc (5.0 4s, 13.3 4p, 81.8 3d)	0.006	0.001	0.007
60	bonding, C4-C9	1.98	50 C4 (29.7 2s, 70.3 2p) 49 C9 (28.9 2s, 71.1 2p)	-0.010	0.000	-0.010
61	bonding, C5-C6	1.95	49 C6 (29.3 2s, 70.7 2p) 49 C5 (29.1 2s, 70.9 2p) 1 Sc (3.9 4s, 11.4 4p, 84.7 3d)	0.011	0.001	0.012
62	bonding, C5-C10	1.98	50 C5 (30.0 2s, 70.0 2p) 49 C1 0(28.6 2s, 71.4 2p)	0.004	0.000	0.004
63	bonding, C6-C11	1.98	50 C6 (30.0 2s, 70.1 2p) 49 C11 (28.9 2s, 71.2 2p)	-0.005	0.000	-0.005
64	bonding, C7-H22	1.98	62 C7 (22.8 2s, 77.2 2p) 37 H22 (100 1s)	-0.004	0.000	-0.004
65	bonding, C7-H23	1.98	61 C7 (22.0 2s, 78.0 2p) 38 H23 (100 1s)	-0.010	0.000	-0.010
66	bonding, C7-H24	1.97	61 C7 (22.0 2s, 78.0 2p) 37 H24 (100 1s)	-0.005	0.000	-0.005
67	bonding, C8-H25	1.97	61 C8 (22.0 2s, 78.0 2p) 38 H25 (100 1s)	-0.003	0.002	-0.001
68	bonding, C8-H26	1.98	61 C8 (22.3 2s, 77.7 2p) 38 H26 (100 1s)	-0.005	0.000	-0.005
69	bonding, C8-H27	1.98	62 C8 (22.8 2s, 77.2 2p) 37 H27 (100 1s)	-0.001	0.000	-0.001
70	bonding, C9-H28	1.98	61 C9 (22.4 2s, 77.6 2p) 38 H28 (100 1s)	-0.012	0.000	-0.012
71	bonding, C9-H29	1.98	61 C9 (22.2 2s, 77.8 2p) 38 H29 (100 1s)	-0.014	0.000	-0.014
72	bonding, C9-H30	1.97	61 C9 (22.0 2s, 78.0 2p) 37 H30 (100 1s)	-0.009	-0.002	-0.011
73	bonding, C10-H31	1.97	61 C10 (21.9 2s, 78.2 2p) 37 H31 (100 1s)	-0.002	0.002	0.000
74	bonding, C10-H32	1.98	61 C10 (22.5 2s, 77.5 2p) 38 H32 (100 1s)	-0.002	0.000	-0.002
75	bonding, C10-H33	1.98	61 C10 (22.3 2s, 77.7 2p) 38 H33 (100 1s)	-0.002	0.000	-0.002
76	bonding, C11-H34	1.97	61 C11 (22.1 2s, 77.9 2p) 37 H34 (100 1s)	-0.007	-0.001	-0.008
77	bonding, C11-H35	1.98	61 C11 (22.1 2s, 77.9 2p) 38 H35 (100 1s)	-0.012	0.000	-0.012
78	bonding, C11-H36	1.98	61 C11 (22.3 2s, 77.7 2p) 38 H36 (100 1s)	-0.007	0.000	-0.007
79	bonding, C12-C13	1.95	49 C13 (29.4 2s, 70.7 2p) 49 C12 (28.8 2s, 71.2 2p) 1 Sc (5.2 4s, 9.4 4p, 85.4 3d)	0.003	0.001	0.004
80	bonding, C12-C16	1.95	49 C16 (29.7 2s, 70.3 2p) 49 C12 (29.6 2s, 70.4 2p)	0.013	0.001	0.014
81	bonding, C12-C17	1.98	51 C12 (30.4 2s, 69.6 2p) 48 C17 (28.5 2s, 71.6 2p)	0.003	0.000	0.003
82	bonding, C13-C14	1.94	49 C14 (28.4 2s, 71.6 2p) 49 C13 (29.2 2s, 70.8 2p) 1 Sc (5.2 4s, 13.1 4p, 81.7 3d)	0.006	0.001	0.007
83	bonding, C13-C18	1.98	50 C13 (29.7 2s, 70.3 2p) 49 C18 (28.9 2s, 71.1 2p)	-0.010	0.000	-0.010
84	bonding, C14-C15	1.95	49 C15 (29.3 2s, 70.7 2p) 49 C14 (29.2 2s, 70.8 2p)	0.012	0.001	0.013
85	bonding, C14-C19	1.98	50 C14 (30. 02s, 70.0 2p) 49 C19 (28.6 2s, 71.4 2p)	0.004	0.000	0.004
86	bonding, C15-C16	1.94	49 C15 (28.8 2s, 71.2 2p) 49 C16 (29.0 2s, 71.0 2p) 1 Sc (6.5 4p, 11.7 4p, 81.8 3d)	0.002	0.001	0.003
87	bonding, C15-C20	1.98	50 C15 (29.9 2s, 70.1 2p) 49 C20 (28.9 2s, 71.2 2p)	-0.005	0.000	-0.005
88	bonding, C16-C21	1.98	51 C16 (30.2 2s, 69.8 2p) 49 C21 (28.6 2s, 71.5 2p)	-0.002	0.000	-0.002

89	bonding, C17-H37	1.98	62 C17 (22.8 2s, 77.2 2p) 37 H37 (100 1s)	-0.001	0.000	-0.001
90	bonding, C17-H38	1.97	61 C17 (22.0 2s, 78.0 2p) 38 H38 (100 1s)	-0.003	0.002	-0.001
91	bonding, C17-H39	1.98	61 C17 (22.3 2s, 77.7 2p) 38 H39 (100 1s)	-0.005	0.000	-0.005
92	bonding, C18-H40	1.98	61 C18 (22.3 2s, 77.8 2p) 38 H40 (100 1s)	-0.014	0.000	-0.014
93	bonding, C18-H41	1.97	61 C18 (22.0 2s, 78.0 2p) 37 H41 (100 1s)	-0.009	-0.002	-0.011
94	bonding, C18-H42	1.98	61 C18 (22.4 2s, 77.6 2p) 38 H42 (100 1s)	-0.013	0.000	-0.013
95	bonding, C19-H43	1.98	61 C19 (22.5 2s, 77.5 2p) 38 H43 (100 1s)	-0.002	0.000	-0.002
96	bonding, C19-H44	1.98	61 C19 (22.2 2s, 77.8 2p) 38 H44 (100 1s)	-0.003	0.000	-0.003
97	bonding, C19-H45	1.97	61 C19 (21.9 2s, 78.1 2p) 37 H45 (100 1s)	-0.002	0.002	0.000
98	bonding, C20-H46	1.97	61 C20 (22.1 2s, 77.9 2p) 37 H46 (100 1s)	-0.006	-0.001	-0.007
99	bonding, C20-H47	1.98	61 C20 (22.2 2s, 77.9 2p) 38 H47 (100 1s)	-0.012	0.000	-0.012
100	bonding, C20-H48	1.98	61 C20 (22.3 2s, 77.7 2p) 38 H48 (100 1s)	-0.007	0.000	-0.007
101	bonding, C21-H49	1.97	61 C21 (22.0 2s, 78.0 2p) 37 H49 (100 1s)	-0.005	0.000	-0.005
102	bonding, C21-H50	1.98	62 C21 (22.9 2s, 77.1 2p) 37 H50 (100 1s)	-0.005	0.000	-0.005
103	bonding, C21-H51	1.98	61 C21 (22.0 2s, 78.0 2p) 38 H51 (100 1s)	-0.010	0.000	-0.010
			Sum of Cp* lone pair / bonding orbital contributions:	**-0.161**	**0.182**	**0.021**
30	core, Br	2.00	100 Br (100 1s)	0.010	0.000	0.010
31	core, Br	2.00	100 Br (100 2s)	0.010	0.000	0.010
32	core, Br	2.00	100 Br (100 3s)	0.011	0.000	0.011
33	core, Br	2.00	100 Br (100 2p)	0.010	0.000	0.010
34	core, Br	2.00	100 Br (100 2p)	0.010	0.000	0.010
35	core, Br	2.00	100 Br (100 2p)	0.010	0.000	0.010
36	core, Br	2.00	100 Br (100 3p)	0.011	0.000	0.011
37	core, Br	2.00	100 Br (100 3p)	0.010	0.000	0.010
38	core, Br	2.00	100 Br (100 3p)	0.010	0.000	0.010
39	core, Br	2.00	100 Br (100 3d)	0.011	0.000	0.011
40	core, Br	2.00	100 Br (100 3d)	0.010	0.000	0.010
41	core, Br	2.00	100 Br (100 3d)	0.010	0.000	0.010
42	core, Br	2.00	100 Br (100 3d)	0.011	0.000	0.011
43	core, Br	2.00	100 Br (100 3d)	0.010	0.000	0.010
			Sum of Br core contributions:	**0.144**	**0.000**	**0.144**
50	lone pair, Br	1.97	99 Br (61.7 4s, 38.4 4p) 1 Sc (10.2 4s, 2.1 4p, 87.7 3d)	0.022	0.010	0.032
51	lone pair, Br	1.92	96 Br (100 4p) 3 Sc (0.7 4p, 99.3 3d)	0.002	0.013	0.015
52	bonding, Sc-Br	1.99	85 Br (38.4 4s, 61.6 4p) 14 Sc (17.5 4s, 0.8 4p, 81.7 3d)	0.137	0.007	0.144
53	bonding, Sc-Br	1.99	92 Br (100 2p) 7 Sc (1.0 4p, 99.1 3d)	-0.027	-0.002	-0.029
			Sum of Br lone pair / bonding contributions:	**0.134**	**0.028**	**0.162**
			Total (0.571 calc'd):	**0.432**	**0.151**	**0.583**

Table S7D. NLMO Contributions to V_{33} (in a.u.) for Cp^*_2ScI

NLMO no.	Orbital Type	Occ.	NLMO Composition	Lewis	non-Lewis	Total
1	core, Sc	2.00	100 Sc (100 1s)	-0.005	0.001	-0.004
2	core, Sc	2.00	100 Sc (100 2s)	-0.007	0.011	0.004
3	core, Sc	2.00	100 Sc (100 3s)	-0.023	-0.053	-0.076
4	core, Sc	2.00	100 Sc (100 2p)	180.216	-0.009	180.207
5	core, Sc	2.00	100 Sc (100 2p)	14.220	-0.011	14.209
6	core, Sc	2.00	100 Sc (100 2p)	177.991	0.002	177.993
7	core, Sc	2.00	100 Sc (100 3p)	14.202	-0.108	14.094
8	core, Sc	2.00	100 Sc (100 3p)	-358.225	0.041	-358.184
9	core, Sc	2.00	100 Sc (100 3p)	-28.078	0.064	-28.014
			Sum of Sc core contributions:	**0.291**	**-0.062**	**0.229**
10	core, C2	2.00	100 C2 (100 1s)	0.006	0.000	0.006
11	core, C3	2.00	100 C3 (100 1s)	0.010	0.000	0.010
12	core, C4	2.00	100 C4 (100 1s)	-0.002	0.000	-0.002
13	core, C5	2.00	100 C5 (100 1s)	0.011	0.000	0.011
14	core, C6	2.00	100 C6 (100 1s)	0.004	0.000	0.004
15	core, C7	2.00	100 C7 (100 1s)	-0.006	0.000	-0.006
16	core, C8	2.00	100 C8 (100 1s)	-0.002	0.000	-0.002
17	core, C9	2.00	100 C9 (100 1s)	-0.012	0.000	-0.012
18	core, C10	2.00	100 C10 (100 1s)	-0.001	0.000	-0.001
19	core, C11	2.00	100 C11 (100 1s)	-0.008	0.000	-0.008
20	core, C12	2.00	100 C12 (100 1s)	0.009	0.000	0.009
21	core, C13	2.00	100 C13 (100 1s)	-0.002	0.000	-0.002
22	core, C14	2.00	100 C14 (100 1s)	0.012	0.000	0.012
23	core, C15	2.00	100 C15 (100 1s)	0.004	0.000	0.004
24	core, C16	2.00	100 C16 (100 1s)	0.007	0.000	0.007
25	core, C17	2.00	100 C17 (100 1s)	-0.003	0.000	-0.003
26	core, C18	2.00	100 C18 (100 1s)	-0.012	0.000	-0.012
27	core, C19	2.00	100 C19 (100 1s)	-0.001	0.000	-0.001
28	core, C20	2.00	100 C20 (100 1s)	-0.009	0.000	-0.009
29	core, C21	2.00	100 C21 (100 1s)	-0.005	0.000	-0.005
			Sum of Cp* core contributions:	**0.000**	**0.000**	**0.000**
53	lone pair, C2	1.08	41 C2 (0.8 2s, 99.2 2p) 40 C3 (0.8 2s, 99.2 2p) 8 Sc (3.9 4s, 0.3 4p, 95.8 3d) 42 C4 (1.2 2s, 98.8 2p)	0.009	0.117	0.126
54	lone pair, C4	1.11	13 Sc (0.1 4s, 0.2 4p, 99.8 2p) 11 C6 (1.1 2s, 98.9 2p) 11 C3 (0.9 2s, 99.1 2p) 7 C2 (0.6 2s, 99.4 2p) 6 C5 (1.8 2s, 98.2 2p)	-0.019	-0.099	-0.118
55	lone pair, C5	1.08	29 C16 (0.7 2s, 99.3 2p) 22 C5 (1.4 2s, 98.6 2p) 10 C12 (0.9 2s, 99.1 2p) 9 C15 (1.3 2s, 98.7 2p) 9 Sc (6.0 4s, 0.2 4p, 93.8 3d) 9 C4 (0.9 2s, 99.1 2p) 7 C6 (1.3 2s, 98.7 2p)	-0.002	0.050	0.048
56	lone pair, C6	1.11	35 C6 (1.4 2s, 98.6 2p) 23 C5 (1.6 2s, 98.4 2p) 17 C16 (0.8 2s, 99.3 2p) 5 C12 (0.9 2s, 99.1 2p) 5 C15 (1.7 2s, 98.3 2p) 5 C2 (1.6 2s, 98.4 2p) 4 Sc (1.1 4s, 1.5 4p, 97.4 3d)	0.001	0.055	0.056
57	lone pair, C13	1.11	48 C13 (1.2 2s, 98.8 2p) 31 C12 (0.9 2s, 99.2 2p) 8 Sc (2.6 4s, 0.4 4p, 96.9 3d) 5 C15 (0.9 2s, 99.1 2p)	-0.025	-0.063	-0.088

58	lone pair, C15	1.11	45 C14 (1.5 2s, 98.6 2p) 34 C15 (1.3 2s, 98.7 2p) 9 Sc (2.5 4s, 0.5 4p, 97.0 3d)	0.005	0.120	0.125
63	bonding, C2-C3	1.95	49 C2 (29.7 2s, 70.3 2p) 49 C3 (29.5 2s, 70.5 2p)	0.013	0.001	0.014
64	bonding, C2-C6	1.94	49 C6 (28.8 2s, 71.2 2p) 49 C2 (28.9 2s, 71.1 2p) 1 Sc (7.8 4s, 11.0 4p, 81.2 3d)	0.003	0.001	0.004
65	bonding, C2-C7	1.98	51 C2 (30.2 2s, 69.8 2p) 48 C7 (28.5 2s, 71.5 2p)	-0.002	0.000	-0.002
66	bonding, C3-C4	1.95	49 C4 (29.3 2s, 70.7 2p) 49 C3 (28.7 2s, 71.3 2p) 1 Sc (6.3 4s, 8.8 4p, 84.9 3d)	0.003	0.001	0.004
67	bonding, C3-C8	1.98	51 C3 (30.4 2s, 69.6 2p) 48 C8 (28.4 2s, 71.7 2p)	0.003	0.000	0.003
68	bonding, C4-C5	1.94	49 C5 (28.4 2s, 71.7 2p) 49 C4 (29.2 2s, 70.8 2p) 1 Sc (6.0 4s, 12.8 4p, 81.2 3d)	0.005	0.001	0.006
69	bonding, C4-C9	1.98	50 C4 (29.7 2s, 70.3 2p) 49 C9 (28.9 2s, 71.1 2p)	-0.010	0.000	-0.010
70	bonding, C5-C6	1.95	49 C6 (29.2 2s, 70.8 2p) 49 C5 (29.1 2s, 70.9 2p) 1 Sc (4.4 4s, 10.9 4p, 84.7 3d)	0.012	0.001	0.013
71	bonding, C5-C10	1.98	50 C5 (30.1 2s, 70.0 2p) 49 C10 (28.6 2s, 71.4 2p)	0.004	0.000	0.004
72	bonding, C6-C11	1.98	50 C6 (29.9 2s, 70.1 2p) 49 C11 (28.8 2s, 71.2 2p)	-0.004	0.000	-0.004
73	bonding, C7-H22	1.98	62 C7 (22.8 2s, 77.2 2p) 37 H22 (100 1s)	-0.005	0.000	-0.005
74	bonding, C7-H23	1.98	61 C7 (22.0 2s, 78.0 2p) 38 H23 (100 1s)	-0.010	0.000	-0.010
75	bonding, C7-H24	1.97	61 C7 (22.1 2s, 77.9 2p) 37 H24 (100 1s)	-0.005	0.000	-0.005
76	bonding, C8-H25	1.97	61 C8 (22.0 2s, 78.0 2p) 38 H25 (100 1s)	-0.003	0.002	-0.001
77	bonding, C8-H26	1.98	61 C8 (22.4 2s, 77.7 2p) 38 H26 (100 1s)	-0.004	0.000	-0.004
78	bonding, C8-H27	1.98	62 C8 (22.8 2s, 77.2 2p) 37 H27 (100 1s)	-0.001	0.000	-0.001
79	bonding, C9-H28	1.98	61 C9 (22.4 2s, 77.6 2p) 38 H28 (100 1s)	-0.013	0.000	-0.013
80	bonding, C9-H29	1.98	61 C9 (22.2 2s, 77.8 2p) 38 H29 (100 1s)	-0.014	0.000	-0.014
81	bonding, C9-H30	1.97	61 C9 (22.1 2s, 78.0 2p) 37 H30 (100 1s)	-0.009	-0.003	-0.012
82	bonding, C10-H31	1.97	61 C10 (21.8 2s, 78.2 2p) 37 H31 (100 1s)	-0.002	0.002	0.000
83	bonding, C10-H32	1.98	61 C10 (22.5 2s, 77.5 2p) 38 H32 (100 1s)	-0.002	0.000	-0.002
84	bonding, C10-H33	1.98	61 C10 (22.3 2s, 77.8 2p) 38 H33 (100 1s)	-0.003	0.000	-0.003
85	bonding, C11-H34	1.97	61 C11 (22.1 2s, 77.9 2p) 37 H34 (100 1s)	-0.006	-0.001	-0.007
86	bonding, C11-H35	1.98	61 C11 (22.1 2s, 77.9 2p) 38 H35 (100 1s)	-0.012	0.000	-0.012
87	bonding, C11-H36	1.98	61 C11 (22.3 2s, 77.7 2p) 38 H36 (100 1s)	-0.007	0.000	-0.007
88	bonding, C12-C13	1.95	49 C13 (29.3 2 s, 70.7 2p) 49 C12 (28.7 2s, 71.3 2p) 1 Sc (6.5 4s, 9.4 4p, 84.1 3d)	0.002	0.001	0.003
89	bonding, C12-C16	1.95	49 C16 (29.8 2s, 70.2 2p) 49 C12 (29.6 70.4 2p)	0.013	0.001	0.014
90	bonding, C12-C17	1.98	51 C12 (30.4 2s, 69.6 2p) 48 C17 (28.4 2s, 71.6 2p)	0.002	0.000	0.002
91	bonding, C13-C14	1.94	49 C14 (28.6 2s, 71.4 2p) 49 C13 (29.2 2s, 70.9 2p) 1 Sc (5.9 4s, 12.7 4p, 81.4 3d)	0.006	0.001	0.007
92	bonding, C13-C18	1.98	50 C13 (29.7 2s, 70.3 2p) 49 C18 (28.9 2s, 71.1 2p)	-0.010	0.000	-0.010
93	bonding, C14-C15	1.95	49 C15 (29.2 2s, 70.9 2p) 49 C14 (29.1 2s, 70.9 2p)	0.011	0.001	0.012
94	bonding, C14-C19	1.98	50 C14 (29.9 2s, 70.1 2p) 49 C19 (28.6 2s, 71.5 2p)	0.004	0.000	0.004
95	bonding, C15-C16	1.94	49 C15(28.9 2s, 71.1 2p) 49 C16 (28.8 2s, 71.2 2p) 1 Sc (7.8 4s, 11.0 4p, 81.3 3d)	0.003	0.001	0.004
96	bonding, C15-C20	1.98	50 C15 (29.9 2s, 70.1 2p) 49 C20 (28.8 2s, 71.2 2p)	-0.005	0.000	-0.005

97	bonding, C16-C21	1.98	51 C16 (30.3 2s, 69.8 2p) 48 C21 (28.5 2s, 71.5 2p)	-0.001	0.000	-0.001
98	bonding, C17-H37	1.98	62 C17 (22.9 2s, 77.1 2p) 37 H37 (100 1s)	-0.002	0.000	-0.002
99	bonding, C17-H38	1.97	61 C17 (21.9 2s, 78.1 2p) 37 H38 (100 1s)	-0.003	0.000	-0.003
100	bonding, C17-H39	1.98	61 C17 (22.3 2s, 77.8 2p) 38 H39 (100 1s)	-0.005	0.000	-0.005
101	bonding, C18-H40	1.98	61 C18 (22.2 2s, 77.8 2p) 38 H40 (100 1s)	-0.014	0.000	-0.014
102	bonding, C18-H41	1.97	61 C18 (22.0 2s, 78.0 2p) 37 H41 (100 1s)	-0.008	-0.001	-0.009
103	bonding, C18-H42	1.98	61 C18 (22.4 2s, 77.6 2p) 38 H42 (100 1s)	-0.012	0.000	-0.012
104	bonding, C19-H43	1.98	61 C19 (22.5 2s, 77.5 2p) 38 H43 (100 1s)	-0.002	0.000	-0.002
105	bonding, C19-H44	1.98	61 C19 (22.3 2s, 77.7 2p) 38 H44 (100 1s)	-0.002	0.000	-0.002
106	bonding, C19-H45	1.97	61 C19 (21.9 2s, 78.1 2p) 37 H45 (100 1s)	-0.002	0.001	-0.001
107	bonding, C20-H46	1.97	61 C20 (22.0 2s, 78.0 2p) 37 H46 (100 1s)	-0.007	0.000	-0.007
108	bonding, C20-H47	1.98	61 C20 (22.1 2s, 77.9 2p) 38 H47 (100 1s)	-0.012	0.000	-0.012
109	bonding, C20-H48	1.98	61 C20 (22.4 2s, 77.7 2p) 38 H48 (100 1s)	-0.007	0.000	-0.007
110	bonding, C21-H49	1.97	61 C21 (21.9 2s, 78.2 2p) 36 H49 (100 1s)	-0.005	0.000	-0.005
111	bonding, C21-H50	1.98	62 C21 (22.8 2s, 77.2 2p) 37 H50 (100 1s)	-0.004	0.000	-0.004
112	bonding, C21-H51	1.98	61 C21 (22.1 2s, 77.9 2p) 38 H51 (100 1s)	-0.009	0.000	-0.009
			Sum of Cp* lone pair / bonding orbital contributions:	**-0.169**	**0.190**	**0.021**
30	core, I	2.00	100 I (100 1s)	0.007	0.000	0.007
31	core, I	2.00	100 I (100 2s)	0.006	0.000	0.006
32	core, I	2.00	100 I (100 3s)	0.007	0.000	0.007
33	core, I	2.00	100 I (100 4s)	0.007	0.000	0.007
34	core, I	2.00	100 I (100 2p)	0.007	0.000	0.007
35	core, I	2.00	100 I (100 2p)	0.007	0.000	0.007
36	core, I	2.00	100 I (100 2p)	0.008	0.000	0.008
37	core, I	2.00	100 I (100 3p)	0.007	0.000	0.007
38	core, I	2.00	100 I (100 3p)	0.006	0.000	0.006
39	core, I	2.00	100 I (100 3p)	0.006	0.000	0.006
40	core, I	2.00	100 I (100 4p)	0.007	0.000	0.007
41	core, I	2.00	100 I (100 4p)	0.006	0.000	0.006
42	core, I	2.00	100 I (100 4p)	0.006	0.000	0.006
43	core, I	2.00	100 I (100 3d)	0.007	0.000	0.007
44	core, I	2.00	100 I (100 3d)	0.007	0.000	0.007
45	core, I	2.00	100 I (100 3d)	0.007	0.000	0.007
46	core, I	2.00	100 I (100 3d)	0.007	0.000	0.007
47	core, I	2.00	100 I (100 3d)	0.006	0.000	0.006
48	core, I	2.00	100 I (100 4d)	0.006	0.000	0.006
49	core, I	2.00	100 I (100 4d)	0.007	0.000	0.007
50	core, I	2.00	100 I (100 4d)	0.007	0.000	0.007
51	core, I	2.00	100 I (100 4d)	0.006	0.000	0.006

52	core, I	2.00	100 I (100 4d)	0.006	0.000	0.006
			Sum of I core contributions:	**0.153**	**0.000**	**0.153**
59	lone pair, I	1.98	99 I (67.1 5s, 32.9 5p) 1 Sc (13.2 4s, 3.4 4p, 83.4 3d)	0.016	0.008	0.024
60	lone pair, I	1.92	96 I (100 5p) 3 Sc (0.6 4p, 99.4 3d)	-0.002	0.013	0.011
61	bonding, Sc-I	1.98	84 I (27.7 5s, 72.3 5p) 16 Sc (18.4 4s, 1.1 4p, 80.5 3d)	0.104	0.014	0.118
62	bonding, Sc-I	1.98	90 I (4.4 5s, 95.7 5p) 9 Sc (5.5 4s, 1.0 4p, 93.5 3d)	-0.010	0.007	-0.003
			Sum of I lone pair / bonding contributions:	**0.108**	**0.042**	**0.150**
			Total (0.547 calc'd):	**0.383**	**0.170**	**0.553**

Table S8A. NLMO Contributions to V_{33} (in a.u.) for $Cp^*_2ScF(THF)$

NLMO no.	Orbital Type	occ	NLMO Composition	Lewis	non-Lewis	Total
1	core, Sc	2.00	100 Sc (100 1s)	-0.001	-0.001	-0.002
2	core, Sc	2.00	100 Sc (100 2s)	-0.008	-0.003	-0.011
3	core, Sc	2.00	100 Sc (100 3s)	0.026	-0.005	0.021
4	core, Sc	2.00	100 Sc (100 2p)	104.848	-0.011	104.837
5	core, Sc	2.00	100 Sc (100 2p)	8.635	-0.018	8.617
6	core, Sc	2.00	100 Sc (100 2p)	177.170	-0.004	177.166
7	core, Sc	2.00	100 Sc (100 3p)	14.755	-0.109	14.646
8	core, Sc	2.00	100 Sc (100 3p)	-282.055	0.016	-282.039
9	core, Sc	2.00	100 Sc (100 3p)	-23.560	0.004	-23.556
			Sum of Sc core contributions:	**-0.190**	**-0.131**	**-0.321**
10	core, C2	2.00	100 C2 (100 1s)	0.014	0.000	0.014
11	core, C3	2.00	100 C3 (100 1s)	0.016	0.000	0.016
12	core, C4	2.00	100 C4 (100 1s)	0.019	0.000	0.019
13	core, C5	2.00	100 C5 (100 1s)	0.000	0.000	0.000
14	core, C6	2.00	100 C6 (100 1s)	-0.008	0.000	-0.008
15	core, C7	2.00	100 C7 (100 1s)	0.003	0.000	0.003
16	core, C8	2.00	100 C8 (100 1s)	-0.007	0.000	-0.007
17	core, C9	2.00	100 C9 (100 1s)	0.015	0.000	0.015
18	core, C10	2.00	100 C10 (100 1s)	0.016	0.000	0.016
19	core, C11	2.00	100 C11 (100 1s)	0.018	0.000	0.018
20	core, C12	2.00	100 C12 (100 1s)	0.005	0.000	0.005
21	core, C13	2.00	100 C13 (100 1s)	0.001	0.000	0.001
22	core, C14	2.00	100 C14 (100 1s)	0.006	0.000	0.006
23	core, C15	2.00	100 C15 (100 1s)	-0.002	0.000	-0.002
24	core, C16	2.00	100 C16 (100 1s)	-0.008	0.000	-0.008
25	core, C17	2.00	100 C17 (100 1s)	-0.002	0.000	-0.002
26	core, C18	2.00	100 C18 (100 1s)	-0.007	0.000	-0.007
27	core, C19	2.00	100 C19 (100 1s)	0.006	0.000	0.006
28	core, C20	2.00	100 C20 (100 1s)	0.001	0.000	0.001
29	core, C21	2.00	100 C21 (100 1s)	0.005	0.000	0.005
			Sum of Cp* core contributions:	**0.091**	**0.000**	**0.091**
36	lone pair, C6	1.14	51 C6 (1.0 2s, 99.1 2p) 10 C4 (0.2 2s, 99.8 2p) 10 C2 (0.7 2s, 99.3 2p) 9 C5 (1.2 2s, 98.8 2p) 8 C3 (0.1 2s, 99.9 2p) 8 Sc (1.1 4s, 0.4 4p, 98.5 3d)	-0.039	-0.076	-0.115
37	lone pair, C7	1.13	50 C7 (0.9 2s, 99.1 2p) 10 C9 (0.4 2s, 99.6 2p) 9 C11 (0.5 2s, 99.5 2p) 9 C8 (1.0 2s, 99.0 2p) 9 Sc (0.6 4s, 0.3 4p, 99.1 3d) 9 C10 (0.1 2s, 99.9 2p)	-0.012	0.029	0.017
44	bonding, C2-C3	1.95	49 C2 (29.8 2s, 70.3 2p) 49 C3 (29.7 2s, 70.3 2p)	0.016	0.001	0.017
45	bonding, C2-C3	1.68	42 C3 (0.3 2s, 99.7 2p) 41 C2 (0.7 2s, 99.3 2p) 7 Sc (1.0 4s, 0.4 4p, 98.7 3d)	0.038	0.050	0.088
46	bonding, C2-C6	1.94	49 C2 (29.2 2s, 70.8 2p) 49 C6 (28.9 2s, 71.1 2p) 1 Sc (10.0 4s, 9.9 4p, 80.1 3d)	0.004	0.001	0.005
47	bonding, C2-C12	1.98	50 C2 (29.4 2s, 70.6 2p) 50 C12 (29.0 2s, 71.0 2p)	0.009	0.000	0.009
48	bonding,	1.94	49 C4 (29.6 2s, 70.4 2p) 49 C3 (29.5 2s, 70.5 2p)	0.018	0.002	0.020

	C3-C4		1 Sc (9.7 4s, 6.0 4p, 84.3 3d)			
49	bonding, C3-C13	1.98	50 C3 (29.8 2s, 70.2 2p) 49 C13 (28.5 2s, 71.5 2p)	0.007	0.000	0.007
50	bonding, C4-C5	1.94	49 C5 (28.4 2s, 71.6 2p) 49 C4 (29.5 2s, 70.5 2p)	0.013	0.001	0.014
51	bonding, C4-C5	1.68	43 C5 (1.2 2s, 98.8 2p) 41 C4 (0.6 2s, 99.4 2p) 7 Sc (1.4 4s, 0.5 4p, 98.1 3d)	0.031	0.069	0.100
52	bonding, C4-C14	1.98	50 C4 (29.7 2s, 70.3 2p) 49 C14 (28.7 2s, 71.3 2p)	0.011	0.000	0.011
53	bonding, C5-C6	1.94	49 C6 (29.6 2s, 70.4 2p) 49 C5 (29.5 2s, 70.5 2p) 1 Sc (9.4 4s, 8.2 4p, 82.4 3d)	-0.008	0.000	-0.008
54	bonding, C5-C15	1.98	50 C5 (29.8 2s, 70.2 2p) 49 C15 (28.6 2s, 71.4 2p)	-0.002	0.000	-0.002
55	bonding, C6-C16	1.98	50 C6 (29.7 2s, 70.4 2p) 49 C16 (29.1 2s, 70.9 2p)	-0.010	0.000	-0.010
56	bonding, C7-C8	1.94	49 C7 (29.0 2s, 71.0 2p) 48 C8 (28.9 2s, 71.1 2p) 1 Sc (8.9 4s, 10.1 4p, 81.0 3d)	-0.006	0.001	-0.005
57	bonding, C7-C11	1.95	49 C7 (29.7 2s, 70.4 2p) 49 C11 (29.7 2s, 70.3 2p) 1 Sc (12.2 4s, 7.3 4p, 80.6 3d)	0.014	0.001	0.015
58	bonding, C7-C17	1.98	50 C7 (29.5 2s, 70.5 2p) 50 C17 (29.0 2s, 71.0 2p)	-0.001	0.000	-0.001
59	bonding, C8-C9	1.94	49 C8 (29.2 2s, 70.8 2p) 49 C9 (29.3 2s, 70.7 2p) 1 Sc (9.9 4s, 8.6 4p, 81.6 3d)	0.004	0.001	0.005
60	bonding, C8-C9	1.68	42 c8 (1.1 2s, 98.9 2p) 41 C9 (0.8 2s, 99.2 2p) 7 Sc (2.1 4s, 0.7 4p, 97.2 3d)	-0.003	0.024	0.021
61	bonding, C8-C18	1.98	50 C8 (29.7 2s, 70.3 2p) 49 C18 (28.7 2s, 71.3 2p)	-0.009	0.000	-0.009
62	bonding, C9-C10	1.94	49 C9 (29.4 2s, 70.6 2p) 48 C10 (29.7 2s, 70.3 2p) 1 Sc (9.9 4s, 7.7 4p, 82.4 3d)	0.019	0.001	0.020
63	bonding, C9-C19	1.98	50 C9 (29.7 2s, 70.3 2p) 49 C19 (28.8 2s, 71.3 2p)	0.010	0.000	0.010
64	bonding, C10-C11	1.95	49 C11 (29.5 2s, 70.5 2p) 48 C10 (29.4 2s, 70.6 2p) 1 Sc (11.0 4s, 5.6 4p, 83.3 3d)	0.016	0.001	0.017
65	bonding, C10-C11	1.68	42 C10 (0.3 2s, 99.7 2p) 42 C11 (0.5 2s, 99.5 2p) 7 Sc (0.5 4s, 0.3 4p, 99.1 3d)	0.037	0.017	0.054
66	bonding, C10-C20	1.98	50 C10 (29.9 2s, 70.1 2p) 49 C20 (28.7 2s, 71.3 2p)	0.006	0.000	0.006
67	bonding, C11-C21	1.98	50 C11 (29.6 2s, 70.4 2p) 49 C21 (28.8 2s, 71.2 2p)	0.010	0.000	0.010
68	bonding, C12-H26	1.98	61 C12 (22.2 2s, 77.8 2p) 39 H26 (100 1s)	0.005	0.000	0.005
69	bonding, C12-H27	1.98	61 C12 (21.9 2s, 78.2 2p) 38 H27 (100 1s)	0.003	0.000	0.003
70	bonding, C12-H28	1.97	61 C12 (21.9 2s, 78.21 2p) 37 H28 (100 1s)	0.004	0.002	0.006
71	bonding, C13-H29	1.98	61 C13 (22.0 2s, 78.0 2p) 39 H29 (100 1s)	0.001	0.000	0.001
72	bonding, C13-H30	1.98	62 C13 (22.5 2s, 77.5 2p) 37 H30 (100 1s)	-0.003	-0.001	-0.004
73	bonding, C13-H31	1.98	61 C13 (22.1 2s, 77.9 2p) 38 H31 (100 1s)	0.001	-0.001	0.000
74	bonding, C14-H32	1.98	62 C14 (22.4 2s, 77.6 2p) 37 H32 (100 1s)	0.003	0.000	0.003
75	bonding C14-H33	1.98	61 C14 (22.2 2s, 77.8 2p) 38 H33 (100 1s)	0.005	0.000	0.005
76	bonding, C14-H34	1.97	61 C14 (22.0 2s, 78.0 2p) 38 H34 (100 1s)	0.004	0.001	0.005
77	bonding, C15-H35	1.98	61 C15 (22.2 2s, 77.8 2p) 38 H35 (100 1s)	0.000	0.000	0.000
78	bonding, C15-H36	1.98	61 C15 (22.3 2s, 77.7 2p) 38 H36 (100 1s)	-0.004	0.000	-0.004
79	bonding, C15-H37	1.97	61 C15 (21.8 2s, 78.2 2p) 38 H37 (100 1s)	-0.001	0.000	-0.001
80	bonding, C16-H38	1.98	61 C16 (22.1 2s, 77.9 2p) 38 H38 (100 1s)	-0.005	-0.001	-0.006
81	bonding, C16-H39	1.98	61 C16 (22.3 2s, 77.8 2p) 38 H39 (100 1s)	-0.009	0.000	-0.009
82	bonding, C16-H40	1.98	60 C16 (21.8 2s, 78.2 2p) 39 H40 (100 1s)	-0.008	0.000	-0.008

83	bonding, C17-H41	1.98	61 C17 (22.1 2s, 77.9 2p) 37 H41 (100 1s)	-0.002	0.000	-0.002
84	bonding, C17-H42	1.98	61 C17 (22.1 2s, 77.9 2p) 38 H42 (100 1s)	0.000	0.000	0.000
85	bonding, C17-H43	1.98	61 C17 (22.1 2s, 77.9 2p) 38 H43 (100 1s)	-0.004	0.000	-0.004
86	bonding, C18-H53	1.98	61C18 (22.3 2s, 77.7 2p) 38 H53 (100 1s)	-0.005	0.000	-0.005
87	bonding, C18-H54	1.98	61 C18 (22.2 2s, 77.8 2p) 38 H54 (100 1s)	-0.010	0.000	-0.010
88	bonding, C18-H55	1.97	61 C19 (22.1 2s, 77.9 2p) 38 H55 (100 1s)	-0.005	-0.001	-0.006
89	bonding, C19-H50	1.98	61 C19 (22.1 2s, 77.9 2p) 38 H50 (100 1s)	0.006	0.001	0.007
90	bonding, C19-H51	1.98	61 C19 (22.0 2s, 78.0 2p) 37 H51 (100 1s)	0.004	0.001	0.005
91	bonding, C19-H52	1.98	61 C19 (22.2 2s, 77.8 2p) 38 H52 (100 1s)	0.003	0.000	0.003
92	bonding, C20-H47	1.98	62 C20 (22.6 2s, 77.4 2p) 37 H47 (100 1s)	-0.003	-0.001	-0.004
93	bonding, C20-H48	1.97	61 C20 (22.0 2s, 78.0 2p) 38 H48 (100 1s)	0.002	-0.001	0.001
94	bonding, C20-H49	1.98	61 C20 (22.0 2s, 78.0 2p) 38 H49 (100 1s)	0.000	0.000	0.000
95	bonding, C21-H44	1.98	61 C21 (22.0 2s, 78.0 2p) 37 H44 (100 1s)	0.003	0.001	0.004
96	bonding, C21-H45	1.98	61 C21 (22.1 2s, 77.9 2p) 38 H45 (100 1s)	0.003	0.000	0.003
97	bonding, C21-H46	1.98	60 C21 (22.1 2s, 77.9 2p) 39 H46 (100 1s)	0.004	0.000	0.004
			Sum of Cp* lone pair / bonding orbital contributions:	**0.165**	**0.123**	**0.288**
34	core, F	2.00	100 F (100 1s)	-0.081	0.000	-0.081
			Sum of F core contributions:	**-0.081**	**0.000**	**-0.081**
38	lone pair, F	1.95	98 F (44.2 2s, 55.8 2p) 2 Sc (19.7 4s, 0.3 4p, 80.0 3d)	-0.092	-0.024	-0.116
39	lone pair, F	1.93	96 F (100 2p) 3 Sc (0.5 4p, 99.5 3d)	-0.058	-0.007	-0.065
40	lone pair, F	1.90	95 F (0.9 2s, 99.1 2p) 5 Sc (0.1 4s, 0.4 4p, 99.6 3d)	-0.058	-0.015	-0.073
41	lone pair, F	1.88	93 F (54.9 2s, 45.1 2p) 6 Sc (3.5 4s, 0.1 4p, 96.4 3d)	-0.237	-0.107	-0.344
			Sum of F lone pair / bonding contributions:	**-0.445**	**-0.153**	**-0.598**
30	core, C22	2.00	100 C22 (100 1s)	0.007	0.000	0.007
31	core, C23	2.00	100 C23 (100 1s)	-0.001	0.000	-0.001
32	core, C24	2.00	100 C24 (100 1s)	0.002	0.000	0.002
33	core, C25	2.00	100 C25 (100 1s)	0.001	0.000	0.001
35	core, O	2.00	100 O (100 1s)	0.022	0.000	0.022
			Sum of THF core contributions:	**0.029**	**0.000**	**0.029**
42	lone pair, O	1.93	97 O (100 2p) 1 Sc (0.1 4s, 1.2 4p, 98.7 3d)	0.018	0.002	0.020
43	lone pair, O	1.88	94 O (41.1 2s, 59.0 2p) 5 Sc (8.5 4s, 0.2 4p, 91.4 3d)	0.056	0.020	0.076
98	bonding, C22-H24	1.98	50 C22 (29.7 2s, 70.3 2p) 49 C24 (25.4 2s, 74.6 2p)	0.004	0.001	0.005
99	bonding, C22-H56	1.97	60 C22 (25.4 2s, 74.6 2p) 38 H56 (100 1s)	0.005	0.000	0.005
100	bonding, C22-H57	1.98	60 C22 (25.5 2s, 74.5 2p) 39 H57 (100 1s)	0.006	0.000	0.006
101	bonding, C22-O65	1.99	69 O (30.1 2s, 69.9 2p) 30 C22 (20.2 2s, 79.8 2p)	0.015	0.001	0.016
102	bonding, C23-C25	1.98	50 C25 (25.8 2s, 74.2 2p) 49 C23 (30.0 2s, 70.0 2p)	0.000	0.001	0.001
103	bonding, C23-H58	1.98	62 C23 (26.3 2s, 73.7 2p) 37 H58 (100 1s)	-0.006	0.000	-0.006
104	bonding,	1.98	60 C23 (25.5 2s, 74.6 2p) 39 H59 (100 1s)	-0.001	0.000	-0.001

	C23-H59					
105	bonding, C23-O65	1.98	70 O (29.7 2s, 70.3 2p) 29 C23 (19.6 2s, 80.4 2p)	0.009	0.001	0.010
106	bonding, C24-C25	1.97	49 C24 (25.9 2s, 74.1 2p) 49 C25 (25.8 2s, 74.2 2p)	0.002	0.000	0.002
107	bonding, C24-H60	1.97	61 C24 (23.2 2s, 76.8 2p) 37 H60 (100 1s)	0.002	0.000	0.002
108	bonding, C24-H61	1.97	61 C24 (22.7 2s, 77.3 2p) 38 H61 (100 1s)	0.002	0.000	0.002
109	bonding, C25-H62	1.97	61 C25 (22.6 2s, 77.5 2p) 38 H62 (100 1s)	0.001	0.000	0.001
110	bonding, C25-H63	1.97	61 C25 (23.1 2s, 76.9 2p) 37 H63 (100 1s)	0.000	0.000	0.000
			Sum of THF lone pair / bonding contributions:	**0.113**	**0.026**	**0.139**
			Total (-0.449 calc'd):	**-0.318**	**-0.135**	**-0.453**

Table S8B. NLMO Contributions to V_{33} (in a.u.) for $Cp^*_2ScCl(THF)$

NLMO no.	Orbital Type	occ	NLMO Composition	Lewis	non-Lewis	Total
1	core, Sc	2.00	100 Sc (100 1s)	-0.001	0.000	-0.001
2	core, Sc	2.00	100 Sc (100 2s)	-0.005	0.001	-0.004
3	core, Sc	2.00	100 Sc (100 3s)	0.018	-0.008	0.010
4	core, Sc	2.00	100 Sc (100 2p)	65.255	-0.007	65.248
5	core, Sc	2.00	100 Sc (100 2p)	5.196	-0.004	5.192
6	core, Sc	2.00	100 Sc (100 2p)	177.570	-0.001	177.569
7	core, Sc	2.00	100 Sc (100 3p)	14.285	-0.102	14.183
8	core, Sc	2.00	100 Sc (100 3p)	-242.845	0.017	-242.828
9	core, Sc	2.00	100 Sc (100 3p)	-19.437	0.020	-19.417
			Sum of Sc core contributions:	**0.036**	**-0.084**	**-0.048**
10	core, C2	2.00	100 C2 (100 1s)	0.014	0.000	0.014
11	core, C3	2.00	100 C3 (100 1s)	0.016	0.000	0.016
12	core, C4	2.00	100 C4 (100 1s)	0.018	0.000	0.018
13	core, C5	2.00	100 C5 (100 1s)	-0.002	0.000	-0.002
14	core, C6	2.00	100 C6 (100 1s)	-0.008	0.000	-0.008
15	core, C7	2.00	100 C7 (100 1s)	0.001	0.000	0.001
16	core, C8	2.00	100 C8 (100 1s)	-0.011	0.000	-0.011
17	core, C9	2.00	100 C9 (100 1s)	0.013	0.000	0.013
18	core, C10	2.00	100 C10 (100 1s)	0.016	0.000	0.016
19	core, C11	2.00	100 C11 (100 1s)	0.017	0.000	0.017
20	core, C12	2.00	100 C12 (100 1s)	0.005	0.000	0.005
21	core, C13	2.00	100 C13 (100 1s)	0.001	0.000	0.001
22	core, C14	2.00	100 C14 (100 1s)	0.006	0.000	0.006
23	core, C15	2.00	100 C15 (100 1s)	-0.004	0.000	-0.004
24	core, C16	2.00	100 C16 (100 1s)	-0.008	0.000	-0.008
25	core, C17	2.00	100 C17 (100 1s)	-0.002	0.000	-0.002
26	core, C18	2.00	100 C18 (100 1s)	-0.008	0.000	-0.008
27	core, C19	2.00	100 C19 (100 1s)	0.005	0.000	0.005
28	core, C20	2.00	100 C20 (100 1s)	0.002	0.000	0.002
29	core, C21	2.00	100 C21 (100 1s)	0.005	0.000	0.005
			Sum of Cp* core contributions:	**0.076**	**0.000**	**0.076**
40	lone pair, C4	1.09	48 C4 (0.7 2s, 99.3 2p) 11 C3 (0.5 2s, 99.5 2p) 11 Sc (0.2 4s, 0.2 4p, 99.7 3d) 10 C6 (0.9 2s, 99.1 2p) 9 C5 (1.2 2s, 98.8 2p) 7 C2 (0.3 2s, 99.7 2p)	0.028	0.073	0.101
41	lone pair, C9	1.06	46 C10 (0.5 2s, 99.5 2p) 11 Sc (0.2 4p, 99.8 3d) 11 C9 (0.7 2s, 99.3 2p) 11 C11 (0.4 2s, 99.6 2p) 10 C7 (0.7 2s, 99.3 2p) 9 C8 (0.9 2s, 99.1 2p)	0.018	-0.032	-0.014
48	bonding, C2-C3	1.95	49 C2 (29.5 2s, 70.5 2p) 49 C3 (29.4 2s, 70.6 2p)	0.016	0.001	0.017
49	bonding, C2-C3	1.67	44 C2 (0.6 2s, 99.4 2p) 39 C3 (0.5 2s, 99.5 2p) 6 Sc (2.4 4s, 0.5 4p, 97.2 3d)	0.035	0.052	0.087
50	bonding, C2-C6	1.94	49 C2 (29.5 2s, 70.5 2p) 49 C6 (29.2 2s, 70.8 2p) 1 Sc (8.1 4s, 8.3 4p, 83.6 3d)	0.005	0.001	0.006
51	bonding, C2-C12	1.98	50 C2 (29.3 2s, 70.7 2p) 50 C12 (29.0 2s, 71.0 2p)	0.009	0.000	0.009
52	bonding,	1.94	49 C4 (29.3 2s, 70.7 2p) 49 C3 (29.2 2s, 70.8 2p)	0.016	0.002	0.018

	C3-C4		1 Sc (9.1 4s, 6.3 4p, 84.6 3d)			
53	bonding, C3-C13	1.98	50 C3 (29.9 2s, 70.1 2p) 49 C13 (28.5 2s, 71.5 2p)	0.007	0.000	0.007
54	bonding, C4-C5	1.94	49 C5 (29.0 2s, 71.0 2p) 49 C4 (29.3 2s, 70.8 2p) 1 Sc (7.9 4s, 9.0 4p, 83.2 3d)	0.010	0.001	0.011
55	bonding, C4-C14	1.98	50 C4 (29.8 2s, 70.2 2p) 49 C14 (28.6 2s, 71.4 2p)	0.011	0.000	0.011
56	bonding, C5-C6	1.94	49 C6 (29.2 2s, 70.8 2p) 49 C5 (28.8 2s, 71.2 2p) 1 Sc (7.9 4s, 8.9 4p, 83.2 3d)	-0.009	0.001	-0.008
57	bonding, C5-C6	1.68	42 C5 (1.2 2s, 98.8 2p) 41.0 C6 (1.1 2s, 98.9 2p)	-0.055	-0.074	-0.129
58	bonding, C5-C15	1.98	50 C5 (29.7 2s, 70.3 2p) 49 C15 (28.5 2s, 71.5 2p)	-0.004	0.000	-0.004
59	bonding, C6-C16	1.98	50 C6 (29.6 2s, 70.4 2p) 49 C16 (28.9 2s, 71.1 2p)	-0.010	0.000	-0.010
60	bonding, C7-C8	1.94	49 C7 (29.1 2s, 70.9 2p) 48 C8 (28.9 2s, 71.1 2p) 1 Sc (6.1 4s, 8.2 4p, 85.7 3d)	-0.010	0.000	-0.010
61	bonding, C7-C8	1.95	49 C7 (29.5 2s, 70.5 2p) 49 C11 (29.5 2s, 70.5 2p) 1 Sc (11.5 4s, 8.5 4p, 80.0 3d)	0.012	0.001	0.013
62	bonding, C7-C11	1.67	43 C7 (0.9 2s, 99.1 2p) 40 C11 (0.4 2s, 99.6 2p) 7 Sc (2.2 4s, 0.5 4p, 97.3 3d)	0.024	0.062	0.086
63	bonding, C7-C17	1.98	49 C17 (28.8 2s, 71.2 2p) 50 C7 (29.5 2s, 70.5 2p)	-0.002	0.000	-0.002
64	bonding, C8-C9	1.94	49 C8 (28.9 2s, 71.1 2p) 49 C9 (29.3 2s, 70.7 2p) 1 Sc (8.3 4s, 8.5 4p, 83.2 3d)	0.001	0.001	0.002
65	bonding, C8-C18	1.68	42 C8 (1.31 2s, 98.7 2p) 41 C9 (0.9 2s, 99.1 2p) 8 Sc (2.5 4s, 0.5 4p, 97.0 3d)	-0.012	0.011	-0.001
66	bonding, C9-C10	1.98	50 C8 (29.7 2s, 70.3 2p) 49 C18 (28.6 2s, 71.4 2p)	-0.012	0.000	-0.012
67	bonding, C9-C19	1.94	49 C9 (29.3 2s, 70.7 2p) 49 C10 (29.2 2s, 70.8 2p) 1 Sc (9.6 4s, 8.4 4p, 82.0 3d)	0.017	0.001	0.018
68	bonding, C10-C11	1.98	50 C9 (29.7 2s, 70.4 2p) 49 C19 (28.7 2s, 71.3 2p)	0.009	0.000	0.009
69	bonding, C10-C11	1.95	49 C11 (29.7 2s, 70.4 2p) 49 C10 (29.3 2s, 70.7 2p) 1 Sc (7.1 4s, 5.2 4p, 87.7 3d)	0.015	0.002	0.017
70	bonding, C10-C20	1.98	51 C10 (30.0 2s, 70.0 2p) 49 C20 (28.6 2s, 71.4 2p)	0.007	0.000	0.007
71	bonding, C11-C21	1.98	50 C11 (29.5 2s, 70.5 2p) 49 C21 (28.8 2s, 71.2 2p)	0.010	0.000	0.010
72	bonding, C12-H26	1.98	61 C12 (22.2 2s, 77.8 2p) 39 H26 (100 1s)	0.005	0.000	0.005
73	bonding, C12-H27	1.98	61 C12 (22.0 2s, 78.1 2p) 38 H27 (100 1s)	0.004	0.000	0.004
74	bonding, C12-H28	1.97	61 C12 (21.8 2s, 78.2 2p) 37 H28 (100 1s)	0.004	0.002	0.006
75	bonding, C13-H29	1.98	60 C13 (21.8 2s, 78.2 2p) 39 H29 (100 1s)	0.000	0.000	0.000
76	bonding, C13-H30	1.98	62 C13 (22.9 2s, 77.1 2p) 37 H30 (100 1s)	-0.002	0.000	-0.002
77	bonding, C13-H31	1.97	61 C13 (22.0 2s, 78.0 2p) 38 H31 (100 1s)	0.002	-0.001	0.001
78	bonding, C14-H32	1.98	62 C14 (22.7 2s, 77.3 2p) 37 H32 (100 1s)	0.004	0.000	0.004
79	bonding, C14-H33	1.98	61 C14 (22.0 2s, 78.0 2p) 38 H33 (100 1s)	0.006	0.000	0.006
80	bonding, C14-H34	1.97	61 C14 (22.0 2s, 78.0 2p) 38 H34 (100 1s)	0.004	0.001	0.005
81	bonding, C15-H35	1.98	61 C15 (22.2 2s, 77.8 2p) 38 H35 (100 1s)	-0.002	0.000	-0.002
82	bonding, C15-H36	1.98	61 C15 (22.4 2s, 77.6 2p) 38 H36 (100 1s)	-0.005	0.000	-0.005
83	bonding, C15-H37	1.97	61 C15 (21.8 2s, 78.2 2p) 37 H37 (100 1s)	-0.002	0.000	-0.002
84	bonding, C16-H38	1.98	61 C16 (22.0 2s, 78.0 2p) 37 H38 (100 1s)	-0.005	-0.001	-0.006
85	bonding, C16-H39	1.98	61 C16 (22.3 2s, 77.7 2p) 38 H39 (100 1s)	-0.009	0.000	-0.009
86	bonding, C16-H40	1.98	60 C16 (21.9 2s, 78.2 2p) 39 H40 (100 1s)	-0.006	0.000	-0.006

87	bonding, C17-H41	1.98	61 C17 (22.0 2s, 78.0 2p) 37 H41 (100 1s)	-0.002	0.000	-0.002
88	bonding, C17-H42	1.98	61 C17 (22.1 2s, 77.9 2p) 38 H42 (100 1s)	0.000	0.000	0.000
89	bonding, C17-H43	1.98	61 C17 (22.2 2s, 77.8 2p) 38 H43 (100 1s)	-0.004	0.000	-0.004
90	bonding, C18-H53	1.98	61 C18 (22.4 2s, 77.6 2p) 38 H53 (100 1s)	-0.006	0.000	-0.006
91	bonding, C18-H54	1.98	61 C18 (22.3 2s, 77.7 2p) 38 H54 (100 1s)	-0.010	0.000	-0.010
92	bonding, C18-H55	1.97	61 C18 (21.7 2s, 78.3 2p) 37 H55 (100 1s)	-0.006	-0.002	-0.008
93	bonding, C19-H50	1.98	61 C19 (22.2 2s, 77.8 2p) 38 H50 (100 1s)	0.006	0.001	0.007
94	bonding, C19-H51	1.97	61 C19 (22.1 2s, 78.0 2p) 37 H51 (100 1s)	0.003	0.001	0.004
95	bonding, C19-H52	1.98	61 C19 (22.2 2s, 77.8 2p) 38 H52 (100 1s)	0.003	0.000	0.003
96	bonding, C20-H47	1.98	62 C20 (22.5 2s, 77.5 2p) 38 H47 (100 1s)	0.000	0.000	0.000
97	bonding, C20-H48	1.97	61 C20 (21.8 2s, 78.2 2p) 38 H48 (100 1s)	0.003	-0.001	0.002
98	bonding, C20-H49	1.98	62 C20 (22.5 2s, 77.5 2p) 37 H49 (100 1s)	0.001	0.000	0.001
99	bonding, C21-H44	1.98	62 C21 (22.2 2s, 77.8 2p) 37 H44 (100 1s)	0.003	0.001	0.004
100	bonding, C21-H45	1.98	61 C21 (22.0 2s, 78.0 2p) 38 H45 (100 1s)	0.003	0.000	0.003
101	bonding, C21-H46	1.98	61 C21 (22.0 2s, 78.0 2p) 39 H46 (100 1s)	0.004	0.000	0.004
			Sum of Cp* lone pair / bonding orbital contributions:	**0.132**	**0.104**	**0.236**
34	core, Cl	2.00	100 Cl (100 1s)	-0.034	0.000	-0.034
35	core, Cl	2.00	100 Cl (100 2s)	-0.034	0.000	-0.034
36	core, Cl	2.00	100 Cl (100 2p)	-0.033	0.000	-0.033
37	core, Cl	2.00	100 Cl (100 2p)	-0.033	0.000	-0.033
38	core, Cl	2.00	100 Cl (100 2p)	-0.034	0.000	-0.034
			Sum of Cl core contributions:	**-0.168**	**0.000**	**-0.168**
42	lone pair, Cl	1.96	98 Cl (52.1 3s, 47.9 3p) 2 Sc (22.0 4s, 0.9 4p, 77.1 3d)	-0.053	-0.019	-0.072
43	lone pair, Cl	1.92	96 Cl (100 3p) 3 Sc (0.7 4p, 99.3 3d)	-0.021	-0.003	-0.024
44	lone pair, Cl	1.87	94 Cl (0.1 3s, 99.9 3p) 6 Sc (0.4 4p, 99.6 3d)	-0.019	-0.011	-0.030
45	lone pair, Cl	1.76	88 Cl (47.7 3s, 62.3 3p) 11 Sc (13.2 4s, 0.7 4p, 86.2 3d)	-0.102	-0.122	-0.224
			Sum of Cl lone pair / bonding contributions:	**-0.195**	**-0.155**	**-0.350**
30	core, C22	2.00	100 C22 (100 1s)	0.007	0.000	0.007
31	core, C23	2.00	100 C23 (100 1s)	-0.003	0.000	-0.003
32	core, C24	2.00	100 C24 (100 1s)	0.002	0.000	0.002
33	core, C25	2.00	100 C25 (100 1s)	0.000	0.000	0.000
39	core, O	2.00	100 O (100 1s)	0.015	0.000	0.015
			Sum of THF core contributions:	**0.021**	**0.000**	**0.021**
46	lone pair, O	1.93	97 O (0.2 2s, 99.8 2p) 1 Sc (0.4 4s, 1.0 4p, 98.6 3d)	0.014	0.002	0.016
47	lone pair, O	1.88	94 O (41.0 2s, 59.0 2p) 5 Sc (9.2 4s, 0.1 4p, 90.7 3d)	0.041	0.016	0.057
102	bonding, C22-C24	1.98	50 C22 (29.7 2s, 70.3 2p) 49 C24 (25.4 2s, 78.6 2p)	0.004	0.001	0.005
103	bonding, C22-H56	1.97	60 C22 (25.5 2s, 74.5 2p) 38 H56 (100 1s)	0.006	0.000	0.006
104	bonding, C22-H57	1.98	60 C22 (25.4 2s, 74.6 2p) 39 H57 (100 1s)	0.006	0.000	0.006

105	bonding, C22-O	1.98	69 O (30.0 2s, 70.0 2p) 30 C22 (20.0 2s, 80.0 2p)	0.012	0.001	0.013
106	bonding, C23-C25	1.98	50 C25 (25.8 2s, 74.2 2p) 49 C23 (30.0 2s, 70.0 2p)	-0.001	0.000	-0.001
107	bonding, C23-H58	1.98	62 C23 (26.3 2s, 73.7 2p) 37 H58 (100 1s)	-0.007	0.000	-0.007
108	bonding, C23-H59	1.98	60 C23 (25.5 2s, 74.5 2p) 39 H59 (100 1s)	-0.003	0.000	-0.003
109	bonding, C23-O	1.98	29 C23 (19.6 2s, 80.4 2p) 70 O (29.8 2s, 70.2 2p)	0.005	0.000	0.005
110	bonding, C24-C25	1.97	49 C24 (25.8 2s, 74.2 2p) 49 C25 (25.8 2s, 74.2 2p)	0.001	0.000	0.001
111	bonding, C24-H60	1.97	61 C24 (23.1 2s, 76.9 2p) 37 H60 (100 1s)	0.001	0.000	0.001
112	bonding, C24-H61	1.97	61 C24 (22.7 2s, 77.3 2p) 38 H61 (100 1s)	0.002	0.000	0.002
113	bonding, C25-H62	1.97	61 C25 (22.5 2s, 77.5 2p) 38 H62 (100 1s)	0.000	0.000	0.000
114	bonding, C25-H63	1.97	61 C25 (23.1 2s, 76.9 2p) 37 H63 (100 1s)	-0.001	0.000	-0.001
			Sum of THF lone pair / bonding contributions:	**0.080**	**0.020**	**0.100**
			Total (-0.137 calc'd):	**-0.018**	**-0.115**	**-0.133**

Table S8C. NLMO Contributions to V_{33} (in a.u.) for $Cp^*_2ScBr(THF)$

NLMO no.	Orbital Type	occ	NLMO Composition	Lewis	non-Lewis	Total
1	core, Sc	2.00	100 Sc (100 1s)	-0.001	0.001	0.000
2	core, Sc	2.00	100 Sc (100 2s)	-0.003	0.004	0.001
3	core, Sc	2.00	100 Sc (100 3s)	-0.008	-0.030	-0.038
4	core, Sc	2.00	100 Sc (100 2p)	-196.518	0.012	-196.506
5	core, Sc	2.00	100 Sc (100 2p)	-15.643	0.018	-15.625
6	core, Sc	2.00	100 Sc (100 2p)	174.854	0.000	174.854
7	core, Sc	2.00	100 Sc (100 3p)	14.019	-0.103	13.916
8	core, Sc	2.00	100 Sc (100 3p)	21.648	0.001	21.649
9	core, Sc	2.00	100 Sc (100 3p)	1.739	-0.008	1.731
			Sum of Sc core contributions:	**0.087**	**-0.105**	**-0.018**
10	core, C2	2.00	100 C2 (100 1s)	0.009	0.000	0.009
11	core, C3	2.00	100 C3 (100 1s)	0.015	0.000	0.015
12	core, C4	2.00	100 C4 (100 1s)	0.001	0.000	0.001
13	core, C5	2.00	100 C5 (100 1s)	0.009	0.000	0.009
14	core, C6	2.00	100 C6 (100 1s)	0.014	0.000	0.014
15	core, C7	2.00	100 C7 (100 1s)	0.011	0.000	0.011
16	core, C8	2.00	100 C8 (100 1s)	0.014	0.000	0.014
17	core, C9	2.00	100 C9 (100 1s)	-0.002	0.000	-0.002
18	core, C10	2.00	100 C10 (100 1s)	0.010	0.000	0.010
19	core, C11	2.00	100 C11 (100 1s)	0.013	0.000	0.013
20	core, C12	2.00	100 C12 (100 1s)	-0.003	0.000	-0.003
21	core, C13	2.00	100 C13 (100 1s)	0.004	0.000	0.004
22	core, C14	2.00	100 C14 (100 1s)	-0.008	0.000	-0.008
23	core, C15	2.00	100 C15 (100 1s)	-0.001	0.000	-0.001
24	core, C16	2.00	100 C16 (100 1s)	0.001	0.000	0.001
25	core, C17	2.00	100 C17 (100 1s)	-0.002	0.000	-0.002
26	core, C18	2.00	100 C18 (100 1s)	0.003	0.000	0.003
27	core, C19	2.00	100 C19 (100 1s)	-0.009	0.000	-0.009
28	core, C20	2.00	100 C20 (100 1s)	0.001	0.000	0.001
29	core, C21	2.00	100 C21 (100 1s)	0.001	0.000	0.001
			Sum of Cp* core contributions:	**0.081**	**0.000**	**0.081**
49	lone pair, C4	1.09	48 C4 (0.7 2s, 99.3 2p) 11 Sc (0.4 4s, 0.2 4p, 99.5 3d) 11 C6 (0.8 2s, 99.2 2p) 10 C3 (0.6 2s, 99.4 2p) 9 C5 (1.2 2s, 98.8 2p) 8 C2 (0.4 2s, 99.6 2p)	-0.023	-0.076	-0.099
50	lone pair, C10	1.06	47 C10 (0.6 2s, 99.4 2p) 11 C9 (0.6 2s, 99.4 2p) 10 C11 (0.4 2s, 99.7 2p) 10 Sc (0.2 4s, 0.2 4p, 99.6 3d) 10 C7 (0.7 2s, 99.3 2p) 9 C8 (0.8 2s, 99.2 2p)	-0.001	0.071	0.070
57	bonding, C2-C3	1.95	49 C2 929.4 2s, 70.6 2p) 49 C3 (29.2 2s, 70. 82p)	0.014	0.001	0.015
58	bonding, C2-C3	1.67	43 C2 (0.6 2s, 99.4 2p) 40 C3 (0.6 2s, 99.4 2p) 7 Sc (2.5 4s, 0.5 4\p, 97.0 3d)	0.021	0.051	0.072
59	bonding, C2-C6	1.94	49 C6 (29.1 2s, 70.9 2p) 49 C2 (29.6 2s, 70.4 2p) 1 Sc (8.5 4s, 7.9 4p, 83.5 3d)	0.010	0.001	0.011
60	bonding, C2-C12	1.98	50 C2 (29.3 2s, 70.7 2p) 49 C12 (28.9 2s, 71.1 2p)	0.000	0.000	0.000
61	bonding,	1.94	49 C4 (29.3 2s, 70.7 2p) 49 C3 (29.5 2s, 70.5 2p)	0.010	0.001	0.011

	C3-C4		1 Sc (9.6 4s, 6.5 4p, 83.9 3d)			
62	bonding, C3-C13	1.98	50 C3 (29.9 2s, 70.1 2p) 49 C13 (28.6 2s, 71.4 2p)	0.009	0.000	0.009
63	bonding, C4-C5	1.94	49 C5 (29.0 2s, 71.0 2p) 49 C4 (29.2 2s, 70.8 2p) 1 Sc (7.8 4s, 8.7 4p, 83.5 3d)	0.003	0.001	0.004
64	bonding, C4-C14	1.98	50 C4 (29.9 2s, 70.2 2p) 49 C14 (28.6 2s, 71.4 2p)	-0.006	0.000	-0.006
65	bonding, C5-C6	1.94	49 C6 (29.3 2s, 70.7 2p) 49 C5 (28.9 2s, 71.1 2p) 1 Sc (7.5 4s, 9.0 4p, 83.5 3d)	0.016	0.001	0.017
66	bonding, C5-C6	1.68	42 C5 (1.2 2s, 98.8 2p) 41 C6 (1.0 2s, 99.0 2p) 7 Sc (2.9 4s, 0.6 4p, 96.5 3d)	0.034	0.087	0.121
67	bonding, C5-C15	1.98	50 C5 (29.7 2s, 70.3 2p) 49 C15 (28.5 2s, 71.5 2p)	0.003	0.000	0.003
68	bonding, C6-C16	1.98	50 C6 (29.6 2s, 70.4 2p) 49 C16 (29.0 2s, 71.1 2p)	0.006	0.000	0.006
69	bonding, C7-C8	1.94	49 C7 (299.2 2s, 70.8 2p) 49 C8 (28.9 2s, 71.1 2p) 1 Sc (6.0 4s, 8.7 4, 85.3 3d)	0.016	0.001	0.017
70	bonding, C7-C11	1.94	49 C7 (29.5 2s, 70.5 2p) 49 C11 (29.5 2s, 70.5 2p) 1 Sc (11.5 4s, 8.4 4p, 80.1 3d)	0.010	0.001	0.011
71	bonding, C7-C11	1.67	43 C7 (1.0 2s, 99.1 2p) 40 C11 (0.4 2s, 99.6 2p) 7 Sc (2.3 4s, 0.5 4p, 97.3 3d)	0.011	-0.018	-0.007
72	bonding, C7-C17	1.98	50 C7 (29.5 2s, 70.5 2p) 49 C17 (28.8 2s, 71.2 2p)	0.002	0.000	0.002
73	bonding, C8-C9	1.94	49 C8 (29.0 2s, 71.0 2p) 49 C9 (29.3 2s, 70.7 2p) 1 Sc (8.3 4s, 8.6 4p, 83.1 3d)	0.007	0.001	0.008
74	bonding, C8-C9	1.68	42 C8 (1.3 2s, 98.7 2p) 41 C9 (0.9 2s, 99.1 2p) 8 Sc (2.6 4s, 0.5 4s, 96.9 3d)	0.000	0.020	0.020
75	bonding, C8-C18	1.98	50 C8 (29.7 2s, 70.3 2p) 49 C18 (28.6 2s, 71.4 2p)	0.007	0.000	0.007
76	bonding, C9-C10	1.94	49 C9 (29.3 2s, 70.7 2p) 49 C10 (29.0 2s, 71.0 2p) 1 Sc (9.5 4s, 8.4 4p, 82.2 3d)	0.002	0.001	0.003
77	bonding, C9-C19	1.98	50 C9 (29.6 2s, 70.4 2p) 49 C19 (28.7 2s, 71.3 2p)	-0.009	0.000	-0.009
78	bonding, C10-C11	1.95	49 C11 (29.7 2s, 70.3 2p) 49 C10 (29.3 2s, 70.7 2p) 1 Sc (7.2 4s, 5.0 4p, 87.8 3d)	0.016	0.001	0.017
79	bonding, C10-C20	1.98	51 C10 (30.1 2s, 69.9 2p) 49 C20 (28.6 2s, 71.4 2p)	0.004	0.000	0.004
80	bonding, C11-C12	1.98	50 C11 (29.6 2s, 70.4 2p) 49 C21 (28.8 2s, 71.2 2p)	0.005	0.000	0.005
81	bonding, C12-H26	1.98	61 C12 (22.2 2s, 77.8 2p) 38 H26 (100 1s)	-0.004	0.000	-0.004
82	bonding, C12-H27	1.98	61 C12 (22.0 2s, 78.0 2p) 39 H27 (100 1s)	-0.005	0.000	-0.005
83	bonding, C12-H28	1.97	61 C12 (21.8 2s, 78.2 2p) 37 H28 (100 1s)	-0.001	-0.001	-0.002
84	bonding, C13-H29	1.98	60 C13 (22.0 2s, 78.0 2p) 38 H29 (100 1s)	0.004	0.000	0.004
85	bonding, C13-H30	1.98	62 C13 (22.8 2s, 77.2 2p) 37 H30 (100 1s)	0.003	0.000	0.003
86	bonding, C13-H31	1.97	61 C13 (21.9 2s, 78.1 2p) 38 H31 (100 1s)	0.002	0.002	0.004
87	bonding, C14-H32	1.98	62 C14 (22.7 2s, 77.3 2p) 37 H32 (100 1s)	-0.007	0.000	-0.007
88	bonding, C14-H33	1.98	61 C14 (22.1 2s, 77.9 2p) 38 H33 (100 1s)	-0.010	0.000	-0.010
89	bonding, C14-H34	1.97	60 C14 (21.9 2s, 78.1 2p) 38 H34 (100 1s)	-0.005	-0.002	-0.007
90	bonding, C15-H35	1.98	61 C15 (22.2 2s, 77.8 2p) 38 H35 (100 1s)	-0.003	0.000	-0.003
91	bonding, C15-H36	1.98	61 C15 (22.5 2s, 77.5 2p) 38 H36 (100 1s)	0.000	0.000	0.000
92	bonding, C15-H37	1.97	61 C15 (21.8 2s, 78.2 2p) 37 H37 (100 1s)	-0.001	0.001	0.000
93	bonding, C16-H38	1.98	61 C16 (22.0 2s, 78.0 2p) 37 H38 (100 1s)	0.001	0.001	0.002
94	bonding, C16-H39	1.98	61 C16 (22.3 2s, 77.7 2p) 38 H39 (100 1s)	0.002	0.000	0.002
95	bonding, C16-H40	1.98	60 C16 (21.9 2s, 78.1 2p) 39 H40 (100 1s)	-0.002	0.000	-0.002

96	bonding, C17-H41	1.98	61 C17 (22.0 2s, 78.0 2p) 37 H41 (100 1s)	-0.001	-0.001	-0.002
97	bonding, C17-H42	1.98	61 C17 (22.1 2s, 77.9 2p) 38 H42 (100 1s)	-0.003	0.000	-0.003
98	bonding, C17-H43	1.98	61 C17 (22.2 2s, 77.8 2p) 38 H43 (100 1s)	-0.003	0.000	-0.003
99	bonding, C18-H53	1.98	61 C18 (22.5 2s, 77.5 2p) 38 H53 (100 1s)	0.001	0.000	0.001
100	bonding, C18-H54	1.98	61 C18 (22.2 2s, 77.8 2p) 38 H54 (100 1s)	0.003	0.000	0.003
101	bonding, C18-H55	1.97	61C18 (21.6 2s, 78.4 2p) 38 H55 (100 1s)	0.002	0.002	0.004
102	bonding, C19-H50	1.98	61 C19 (22.2 2s, 77.8 2p) 38 H50 (100 1s)	-0.012	-0.001	-0.013
103	bonding, C19-H51	1.97	61 C19 (22.0 2s, 78.0 2p) 37 H51 (100 1s)	-0.006	-0.002	-0.008
104	bonding, C19-H52	1.98	61 C19 (22.3 2s, 77.8 2p) 38 H52 (100 1s)	-0.008	0.000	-0.008
105	bonding, C20-H47	1.98	62 C20 (22.5 2s, 77.5 2p) 38 H47 (100 1s)	0.002	0.000	0.002
106	bonding, C20-H48	1.97	61 C20 (21.9 2s, 78.1 2p) 38 H48 (100 1s)	0.000	0.001	0.001
107	bonding, C20-H49	1.98	62 C20 (22.5 2s, 77.5 2p) 37 H49 (100 1s)	-0.002	0.000	-0.002
108	bonding, C21-H44	1.98	61 C21 (22.1 2s, 77.9 2p) 37 H44 (100 1s)	0.001	0.000	0.001
109	bonding, C21-H45	1.98	61 C21 (22.2 2s, 77.9 2p) 38 H45 (100 1s)	0.001	0.000	0.001
110	bonding, C21-H46	1.98	61 C21 (22.0 2s, 78.0 2p) 39 H46 (100 1s)	-0.002	0.000	-0.002
			Sum of Cp* lone pair / bonding orbital contributions:	**0.103**	**0.144**	**0.247**
34	core, Br	2.00	100 Br (100 1s)	0.006	0.000	0.006
35	core, Br	2.00	100 Br (100 2s)	0.006	0.000	0.006
36	core, Br	2.00	100 Br (100 3s)	0.006	0.000	0.006
37	core, Br	2.00	100 Br (100 2p)	0.006	0.000	0.006
38	core, Br	2.00	100 Br (100 2p)	0.006	0.000	0.006
39	core, Br	2.00	100 Br (100 2p)	0.006	0.000	0.006
40	core, Br	2.00	100 Br (100 3p)	0.006	0.000	0.006
41	core, Br	2.00	100 Br (100 3p)	0.006	0.000	0.006
42	core, Br	2.00	100 Br (100 3p)	0.007	0.000	0.007
43	core, Br	2.00	100 Br (100 3d)	0.006	0.000	0.006
44	core, Br	2.00	100 Br (100 3d)	0.006	0.000	0.006
45	core, Br	2.00	100 Br (100 3d)	0.006	0.000	0.006
46	core, Br	2.00	100 Br (100 3d)	0.006	0.000	0.006
47	core, Br	2.00	100 Br (100 3d)	0.006	0.000	0.006
			Sum of Br core contributions:	**0.085**	**0.000**	**0.085**
51	lone pair, Br	1.97	98 Br (60.9 4s, 39.1 4p) 1 Sc (21.8 4s, 2.1 4p, 76.1 3d)	0.012	0.007	0.019
52	lone pair, Br	1.92	96 Br (100 4p) 3 Sc (0.7 4p, 99.3 3d)	0.001	0.010	0.011
53	lone pair, Br	1.87	94 Br (100 2p) 6 Sc (0.4 4p, 99.5 3d)	0.006	-0.021	-0.015
54	lone pair, Br	1.73	85 Br (39.1 4s, 60.9 4p) 14 Sc (13.2 4s, 0.9 4p, 86.0 3d)	0.016	0.058	0.074
			Sum of Br lone pair / bonding contributions:	**0.035**	**0.054**	**0.089**
30	core, C22	2.00	100 C22 (100 1s)	-0.018	0.000	-0.018
31	core, C23	2.00	100 C23 (100 1s)	-0.006	0.000	-0.006
32	core, C24	2.00	100 C24 (100 1s)	-0.008	0.000	-0.008

33	core, C25	2.00	100 C25 (100 1s)	-0.005	0.000	-0.005
48	core, O	2.00	100 O (100 1s)	-0.038	0.000	-0.038
			Sum of THF core contributions:	**-0.075**	**0.000**	**-0.075**
55	lone pair, O	1.93	97 O (0.2 2s, 99.8 2p) 1 Sc (0.3 4s, 1.0 4p, 98.7 3d)	-0.031	0.000	-0.031
56	lone pair, O	1.88	94 O (41.3 2s, 58.7 2p) 5 Sc (9.6 4s, 0.1 4p, 90.3 3d)	-0.100	-0.036	-0.136
111	bonding, C22-C24	1.98	50 C22 (29.7 2s, 70.3 2p) 49 C24 (25.4 2s, 74.6 2p)	-0.011	-0.001	-0.012
112	bonding, C22-H56	1.97	60 C22 (25.5 2s, 74.5 2p) 38 H56 (100 1s)	-0.017	-0.001	-0.018
113	bonding, C22-H57	1.98	60 C22 (25.5 2s, 74.6 2p) 38 H57 (100 1s)	-0.014	0.000	-0.014
114	bonding, C22-O	1.98	69 O (29.9 2s, 70.1 2p) 30 C22 (20.0 2s, 80.0 2p)	-0.030	-0.002	-0.032
115	bonding, C23-C25	1.98	50 C25 (25.7 2s, 74.3 2p) 49 C23 (30.0 2s, 70.0 2p)	-0.006	-0.001	-0.007
116	bonding, C23-H58	1.98	62 C23 (26.4 2s, 73.6 2p) 37 H58 (100 1s)	-0.002	0.000	-0.002
117	bonding, C23-H59	1.98	60 C23 (25.5 2s, 74.5 2p) 39 H59 (100 1s)	-0.003	0.000	-0.003
118	bonding, C23-O	1.98	70 O (29.6 2s, 70.4 2p) 29 C23 (19.7 2s, 80.3 2p)	-0.024	-0.001	-0.025
119	bonding, C24-C25	1.97	49 C24 (25.8 2s, 74.2 2p) 49 C25 (25.9 2s, 74.1 2p)	-0.006	0.000	-0.006
120	bonding, C24-H60	1.97	61 C24 (23.1 2s, 76.9 2p) 37 H60 (100 1s)	-0.006	0.000	-0.006
121	bonding, C24-H61	1.97	61 C24 (22.7 2s, 77.3 2p) 38 H61 (100 1s)	-0.007	0.000	-0.007
122	bonding, C25-H62	1.97	61 C25 (22.5 2s, 77.5 2p) 38 H62 (100 1s)	-0.005	0.000	-0.005
123	bonding, C25-H63	1.97	61 C25 (23.1 2s, 76.9 2p) 37 H63 (100 1s)	-0.004	-0.001	-0.005
			Sum of THF lone pair / bonding contributions:	**-0.266**	**-0.043**	**-0.309**
			Total (0.113 calc'd):	**0.061**	**0.051**	**0.112**

Table S8D. NLMO Contributions to V_{33} (in a.u.) for $Cp^*_2ScI(THF)$

NLMO no.	Orbital Type	occ	NLMO Composition	Lewis	non-Lewis	Total
1	core, Sc	2.00	100 Sc (100 1s)	-0.001	0.001	0.000
2	core, Sc	2.00	100 Sc (100 2s)	-0.003	0.004	0.001
3	core, Sc	2.00	100 Sc (100 3s)	-0.005	-0.029	-0.034
4	core, Sc	2.00	100 Sc (100 2p)	-10.163	0.002	-10.161
5	core, Sc	2.00	100 Sc (100 2p)	-0.810	-0.003	-0.813
6	core, Sc	2.00	100 Sc (100 2p)	-167.545	0.014	-167.531
7	core, Sc	2.00	100 Sc (100 3p)	-13.286	0.010	-13.276
8	core, Sc	2.00	100 Sc (100 3p)	177.696	0.001	177.697
9	core, Sc	2.00	100 Sc (100 3p)	14.229	-0.103	14.126
			Sum of Sc core contributions:	**0.112**	**-0.103**	**0.009**
10	core, C2	2.00	100 C2 (100 1s)	0.008	0.000	0.008
11	core, C3	2.00	100 C3 (100 1s)	0.015	0.000	0.015
12	core, C4	2.00	100 C4 (100 1s)	0.002	0.000	0.002
13	core, C5	2.00	100 C5 (100 1s)	0.013	0.000	0.013
14	core, C6	2.00	100 C6 (100 1s)	0.012	0.000	0.012
15	core, C7	2.00	100 C7 (100 1s)	0.007	0.000	0.007
16	core, C8	2.00	100 C8 (100 1s)	0.016	0.000	0.016
17	core, C9	2.00	100 C9 (100 1s)	0.003	0.000	0.003
18	core, C10	2.00	100 C10 (100 1s)	0.011	0.000	0.011
19	core, C11	2.00	100 C11 (100 1s)	0.012	0.000	0.012
20	core, C12	2.00	100 C12 (100 1s)	-0.003	0.000	-0.003
21	core, C13	2.00	100 C13 (100 1s)	0.004	0.000	0.004
22	core, C14	2.00	100 C14 (100 1s)	-0.007	0.000	-0.007
23	core, C15	2.00	100 C15 (100 1s)	0.001	0.000	0.001
24	core, C16	2.00	100 C16 (100 1s)	0.000	0.000	0.000
25	core, C17	2.00	100 C17 (100 1s)	-0.003	0.000	-0.003
26	core, C18	2.00	100 C18 (100 1s)	0.004	0.000	0.004
27	core, C19	2.00	100 C19 (100 1s)	-0.007	0.000	-0.007
28	core, C20	2.00	100 C20 (100 1s)	0.001	0.000	0.001
29	core, C21	2.00	100 C21 (100 1s)	0.001	0.000	0.001
			Sum of Cp* core contributions:	**0.090**	**0.000**	**0.090**
58	lone pair, C3	1.07	49 C3 (0.6 2s, 99.4 2p) 12 C2 (0.6 2s, 99.4 2p) 11 C4 (0.6 2s, 99.4 2p) 10 Sc (0.6 4s, 0.2 4p, 99.2 3d) 8 C6 (0.7 2s, 99.3 2p) 7 C5 (0.6 2s, 99.4 2p)	0.012	0.125	0.137
59	lone pair, C10	1.07	47 C10 (0.7 2s, 99.3 2p) 11 C9 (0.7 2s, 99.3 2p) 11 Sc (0.2 4s, 0.2 4p, 99.6 3d) 10 C7 (0.7 2s, 99.3 2p) 10 C11 (0.3 2s, 99.7 2p) 9 C8 (0.7 2s, 99.3 2p)	0.001	0.056	0.057
66	bonding, C2-C3	1.95	49 C2 (29.7 2s, 70.3 2p) 49 C3 (29.3 2s, 70.7 2p) 1 Sc (8.0 4s, 5.6 4p, 86.4 3d)	0.015	0.001	0.016
67	bonding, C2-C6	1.94	49 C2 (29.1 2s, 70.9 2p) 49 C6 (28.8 2s, 71.2 2p) 1 Sc (9.4 4s, 10.8 4p, 79.8 3d)	0.008	0.001	0.009
68	bonding, C2-C6	1.68	44 C6 (1.1 2s, 99.0 2p) 39 C2 (0.7 2s, 99.3 2p) 7 Sc (2.2 4s, 0.5 4p, 97.3 3d)	0.004	-0.028	-0.024
69	bonding, C2-C12	1.98	50 C2 (29.4 2s, 70.6 2p) 49 C12 (28.9 2s, 71.1 2p)	0.001	0.000	0.001
70	bonding, C3-	1.94	49 C3 (29.2 2s, 70.8 2p) 49 C4 (29.5 2s, 70.5 2p)	0.010	0.001	0.011

	C4		1 Sc (11.0 4s, 6.1 4p, 83.0 3d)			
71	bonding, C3-C13	1.98	51 C3 (30.0 2s, 70.0 2p) 49 C13 (28.5 2s, 71.5 2p)	0.009	0.000	0.009
72	bonding, C4-C5	1.94	49 C5(28.4 2s, 71.6 2p) 49 C4 (29.1 2s, 70. 9 2p) 1 Sc (8.4 4s, 9.6 4p, 82.0 3d)	0.006	0.001	0.007
73	bonding, C4-C5	1.68	44 C5 (1.1 2s, 98.9 2p) 39 C4 (0.8 2s, 99.2 2p) 7 Sc (2.4 4s, 0.5 4p, 97.1 3d)	-0.005	-0.013	-0.018
74	bonding, C4-C14	1.98	51 C4 (29.8 2s, 70.2 2p) 49 C14 (28.5 2s, 71.5 2p)	-0.005	0.000	-0.005
75	bonding, C5-C6	1.94	49 C6 (29.6 2s, 70.4 2p) 48 C5 (29.5 2s, 70.5 2p) 1 Sc (7.3 4s, 7.0 4p, 85.8 3d)	0.018	0.001	0.019
76	bonding, C5-C15	1.98	50 C5 (29.8 2s, 70.2 2p) 49 C15 (28.5 2s, 71.5 2p)	0.005	0.000	0.005
77	bonding, C6-C16	1.98	50 C6 (29.6 2s, 70.4 2p) 49 C16 (28.9 2s, 71.1 2p)	0.004	0.000	0.004
78	bonding, C7-C8	1.94	49 C7 (29.2 2s, 70.8 2p) 49 C8 (28.9 2s, 71.1 2p) 1 Sc (5.9 4s, 8.5 4p, 85.6 3d)	0.015	0.001	0.016
79	bonding, C7-C11	1.95	49 C7 (29.4 2s, 70.6 2p) 49 C11 (29.5 2s, 70.5 2p) 1 Sc (13.0 4s, 8.2 4p, 78.8 3d)	0.008	0.001	0.009
80	bonding, C7-C11	1.67	43 C7 (1.0 2s, 99.0 2p) 40 C11 (0.4 2s, 99.6 2p) 7 Sc (2.5 4s, 0.4 4p, 97.1 3d)	0.000	-0.020	-0.020
81	bonding, C7-C17	1.98	50 C7 (29.5 2s, 70.5 2p) 49 C17 (28.8 2s, 71.2 2p)	-0.001	0.000	-0.001
82	bonding, C8-C9	1.94	49 C8 (28.9 2s, 71.1 2p) 49 C9 (29.4 2s, 70.6 2p) 1 Sc (9.1 4s, 8.4 4p, 82.5 3d)	0.011	0.001	0.012
83	bonding, C8-C9	1.68	42 C8 (1.3 2s, 98.7 2p) 41 C9 (0.8 2s, 99.2 2p) 8 Sc (2.6 2s, 0.5 4p, 96.9 3d)	0.014	0.043	0.057
84	bonding, C8-C18	1.98	50 C8 (29.7 2s, 70.3 2p) 49 C18 (28.5 2s, 71.5 2p)	0.009	0.000	0.009
85	bonding, C9-C10	1.94	49 C9 (29.3 2s, 70.7 2p) 49 C10 (29.0 2s, 71.0 2p) 1 Sc (10.8 4s, 8.3 4p, 80.9 3d)	0.005	0.001	0.006
86	bonding, C9-C19	1.98	50 C9 (29.6 2s, 70.4 2p) 49 C19 (28.6 2s, 71.4 2p)	-0.005	0.000	-0.005
87	bonding, C10-C11	1.95	49 C11 (29.8 2s, 70.2 2p) 49 C10 (29.2 2s, 70.8 2p) 1 Sc (7.8 4s, 5.0 4p, 87.3 3d)	0.016	0.001	0.017
88	bonding, C10-C20	1.98	51 C10 (30.1 2s, 69.9 2p) 48 C20 (28.4 2s, 71.6 2p)	0.005	0.000	0.005
89	bonding, C11-C21	1.98	50 C11 (29.5 2s, 70.5 2p) 49 C21 (28.7 2s, 71.3 2p)	0.005	0.000	0.005
90	bonding, C12-H26	1.98	61 C12 (22.2 2s, 77.8 2p) 38 H26 (100 1s)	-0.003	0.000	-0.003
91	bonding, C12-H27	1.98	61 C12 (22.1 2s, 78.0 2p) 38 H27 (100 1s)	-0.005	0.000	-0.005
92	bonding, C12-H28	1.97	61 C12 (21.8 2s, 78.2 2p) 37 H28 (100 1s)	-0.001	-0.001	-0.002
93	bonding, C13-H29	1.98	61 C13 (22.0 2s, 78.0 2p) 38 H29 (100 1s)	0.004	0.000	0.004
94	bonding, C13-H30	1.98	62 C13 (22.9 2s, 77.1 2p) 37 H30 (100 1s)	0.002	0.000	0.002
95	bonding, C13-H31	1.97	61 C13 (21.9 2s, 78.1 2p) 38 H31 (100 1s)	0.002	0.002	0.004
96	bonding, C14-H32	1.98	62 C14 (22.8 2s, 77.2 2p) 37 H32 (100 1s)	-0.007	0.000	-0.007
97	bonding, C14-H33	1.98	61 C14 (22.1 2s, 77.9 2p) 38 H33 (100 1s)	-0.009	0.000	-0.009
98	bonding, C14-H34	1.97	61 C14 (21.9 2s, 78.1 2p) 38 H34 (100 1s)	-0.004	-0.002	-0.006
99	bonding, C15-H35	1.98	61 C15 (22.2 2s, 77.8 2p) 38 H35 (100 1s)	-0.001	0.000	-0.001
100	bonding, C15-H36	1.98	61 C15 (22.5 2s, 77.5 2p) 38 H36 (100 1s)	0.002	0.000	0.002
101	bonding, C15-H37	1.97	61 C15 (21.8 2s, 78.2 2p) 37 H37 (100 1s)	0.001	0.001	0.002
102	bonding, C16-H38	1.97	61 C16 (22.0 2s, 78.0 2p) 37 H38 (100 1s)	0.000	0.000	0.000
103	bonding, C16-H39	1.98	61 C16 (22.3 2s, 77.7 2p) 38 H39 (100 1s)	0.001	0.000	0.001
104	bonding, C16-H40	1.98	60 C16 (21.9 2s, 78.1 2p) 39 H40 (100 1s)	-0.003	0.000	-0.003

105	bonding, C17-H41	1.98	61 C17 (22.0 2s, 78.0 2p) 37 H41 (100 1s)	-0.002	-0.001	-0.003
106	bonding, C17-H42	1.98	61 C17 (22.1 2s, 77.9 2p) 37 H41 (100 1s)	-0.004	0.000	-0.004
107	bonding, C17-H43	1.98	61 C17 (22.2 2s, 77.8 2p) 38 H43 (100 1s)	-0.005	0.000	-0.005
108	bonding, C18-H53	1.98	61 C18 (22.5 2s, 77.5 2p) 38 H53 (100 1s)	0.002	0.000	0.002
109	bonding, C18-H54	1.98	61 C18 (22.3 2s, 77.7 2p) 38 H54 (100 1s)	0.004	0.000	0.004
110	bonding, C18-H55	1.97	61 C18 (21.7 2s, 78.3 2p) 37 H55 (100 1s)	0.003	0.002	0.005
111	bonding, C19-H50	1.98	62 C19 (22.3 2s, 77.7 2p) 37 H50 (100 1s)	-0.010	0.000	-0.010
112	bonding, C19-H51	1.97	61 C19 (22.0 2s, 78.0 2p) 37 H51 (100 1s)	-0.004	-0.002	-0.006
113	bonding, C19-H52	1.98	61 C19 (22.2 2s, 77.8 2p) 38 H52 (100 1s)	-0.006	0.000	-0.006
114	bonding, C20-H47	1.98	62 C20 (22.5 2s, 77.5 2p) 37 H47 (100 1s)	0.002	0.000	0.002
115	bonding, C20-H48	1.97	61 C20 (21.8 2s, 78.2 2p) 38 H48 (100 1s)	0.001	0.001	0.002
116	bonding, C20-H49	1.98	62 C20 (22.6 2s, 77.4 2p) 37 H49 (100 1s)	-0.002	0.000	-0.002
117	bonding, C21-H44	1.98	62 C21 (22.2 2s ,77.8 2p) 37 H44 (100 1s)	0.001	0.000	0.001
118	bonding, C22-H45	1.98	61 C21 (22.0 2s, 78.0 2p) 38 H45 (100 1s)	0.002	0.000	0.002
119	bonding, C22-H46	1.98	61 C21 (22.1 2s, 77.9 2p) 38 H46 (100 1s)	-0.001	0.000	-0.001
			Sum of Cp* lone pair / bonding orbital contributions:	**0.125**	**0.173**	**0.298**
34	core, I	2.00	100 I (100 1s)	0.000	0.000	0.000
35	core, I	2.00	100 I (100 2s)	0.000	0.000	0.000
36	core, I	2.00	100 I (100 3s)	0.000	0.000	0.000
37	core, I	2.00	100 I (100 4s)	0.000	0.000	0.000
38	core, I	2.00	100 I (100 2p)	0.000	0.000	0.000
39	core, I	2.00	100 I (100 2p)	0.000	0.000	0.000
40	core, I	2.00	100 I (100 2p)	-0.001	0.000	-0.001
41	core, I	2.00	100 I (100 3p)	0.000	0.000	0.000
42	core, I	2.00	100 I (100 3p)	0.000	0.000	0.000
43	core, I	2.00	100 I (100 3p)	0.000	0.000	0.000
44	core, I	2.00	100 I (100 4p)	0.000	0.000	0.000
45	core, I	2.00	100 I (100 4p)	0.000	0.000	0.000
46	core, I	2.00	100 I (100 4p)	0.000	0.000	0.000
47	core, I	2.00	100 I (100 3d)	0.000	0.000	0.000
48	core, I	2.00	100 I (100 3d)	-0.001	0.000	-0.001
49	core, I	2.00	100 I (100 3d)	0.000	0.000	0.000
50	core, I	2.00	100 I (100 3d)	-0.001	0.000	-0.001
51	core, I	2.00	100 I (100 3d)	0.000	0.000	0.000
52	core, I	2.00	100 I (100 4d)	0.000	0.000	0.000
53	core, I	2.00	100 I (100 4d)	0.000	0.000	0.000
54	core, I	2.00	100 I (100 4d)	0.000	0.000	0.000
55	core, I	2.00	100 I (100 4d)	0.000	0.000	0.000
56	core, I	2.00	100 I (100 4d)	0.000	0.000	0.000

			Sum of I core contributions:	**-0.003**	**0.000**	**-0.003**
60	lone pair, I	1.97	99 I (67.4 5s, 32.6 5p) 1 Sc (26.5 4s, 3.3 4p, 70.2 3d)	0.001	0.003	0.004
61	lone pair, I	1.92	96 I (100 5p) 3 Sc (0.6 4p, 99.4 3d)	-0.002	0.007	0.005
62	lone pair, I	1.88	94 I (0.1 5s, 99.9 5p) 5 Sc (0.4 4p, 99.6 3d)	0.003	-0.019	-0.016
63	lone pair, I	1.67	82 I (32.6 5s, 67.4 5p) 17 Sc (15.5 4s, 1.2 4p, 83.3 3d)	-0.003	0.028	0.025
			Sum of I lone pair / bonding contributions:	**-0.001**	**0.019**	**0.018**
30	core, C22	2.00	100 C22 (100 1s)	-0.017	0.000	-0.017
31	core, C23	2.00	100 C23 (100 1s)	-0.002	0.000	-0.002
32	core, C24	2.00	100 C24 (100 1s)	-0.006	0.000	-0.006
33	core, C25	2.00	100 C25 (100 1s)	-0.004	0.000	-0.004
57	core, O	2.00	100 O (100 1s)	-0.028	0.000	-0.028
			Sum of THF core contributions:	**-0.057**	**0.000**	**-0.057**
64	lone pair, O	1.93	97 O (0.3 2s, 99.8 2p) 1 Sc (0.5 4s, 1.0 4p, 98.5 3d)	-0.022	0.000	-0.022
65	lone pair, O	1.88	94 O (41.0 2s, 59.0 2p) 5 Sc (9.5 4s, 0.1 4p, 90.4 3d)	-0.071	-0.025	-0.096
120	bonding, C22-C24	1.98	50 C22 (29.7 2s, 70.3 2p) 49 C24 (25.4 2s, 74.6 2p)	-0.010	-0.001	-0.011
121	bonding, C22-H56	1.97	60 C22 (25.5 2s, 74.5 2p) 38 H56 (100 1s)	-0.017	-0.001	-0.018
122	bonding, C22-H57	1.98	60 C22 (25.4 2s, 74.6 2p) 38 H57 (100 1s)	-0.013	0.000	-0.013
123	bonding, C22-O	1.98	69 O (29.9 2s, 70.1 2p) 30 C22 (19.9 2s, 80.1 2p)	-0.024	-0.001	-0.025
124	bonding, C23-C25	1.98	50 C25 (25.8 2s, 74.3 2p) 49 C23 (30.0 2s, 70.0 2p)	-0.004	-0.001	-0.005
125	bonding, C23-H58	1.98	62 C23 (26.5 2s, 73.5 2p) 37 H58 (100 1s)	0.001	0.000	0.001
126	bonding, C23-H59	1.98	60 C23 (25.4 2s, 74.6 2p) 39 H591 (100 1s)	0.000	0.000	0.000
127	bonding, C23-O	1.99	70 O (29.8 2s, 70.2 2p) 29 C23 (19.6 2s, 80.5 2p)	-0.016	-0.001	-0.017
128	bonding, C24-C25	1.97	49 C24 (25.8 2s, 74.2 2p) 49 C25 (25.9 2s, 74.1 2p)	-0.005	0.000	-0.005
129	bonding, C24-H60	1.97	61 C24 (23.1 2s, 76.9 2p) 37 H60 (100 1s)	-0.005	0.000	-0.005
130	bonding, C24-H61	1.97	61 C24 (22.7 2s, 77.3 2p) 38 H61 (100 1s)	-0.006	0.000	-0.006
131	bonding, C25-H62	1.97	61 C25 (22.5 2s, 77.5 2p) 38 H62 (100 1s)	-0.003	0.000	-0.003
132	bonding, C25-H63	1.97	61 C25 (23.1 2s, 76.9 2p) 37 H63 (100 1s)	-0.003	-0.001	-0.004
			Sum of THF lone pair / bonding contributions:	**-0.198**	**-0.031**	**-0.229**
			Total (0.113 calc'd):	**0.068**	**0.058**	**0.126**

Geometry Optimized Coordinates:

Cp^*_2ScF

1 Sc	0.000000000000	-0.473000000000	-0.002000000000
2 C	2.251000000000	-0.571000000000	0.953000000000
3 C	2.400000000000	-0.859000000000	-0.430000000000
4 C	2.042000000000	0.309000000000	-1.162000000000
5 C	1.727000000000	1.340000000000	-0.226000000000
6 C	1.832000000000	0.790000000000	1.083000000000
7 C	2.490000000000	-1.552000000000	2.066000000000
8 H	2.044000000000	-2.525000000000	1.835000000000
9 H	2.065000000000	-1.202000000000	3.012000000000
10 H	3.562000000000	-1.712000000000	2.234000000000
11 C	2.839000000000	-2.181000000000	-0.986000000000
12 H	3.892000000000	-2.377000000000	-0.747000000000
13 H	2.742000000000	-2.211000000000	-2.075000000000
14 H	2.237000000000	-2.996000000000	-0.575000000000
15 C	2.099000000000	0.482000000000	-2.656000000000
16 H	1.347000000000	1.194000000000	-3.010000000000
17 H	1.933000000000	-0.463000000000	-3.181000000000
18 H	3.078000000000	0.862000000000	-2.978000000000
19 C	1.561000000000	2.788000000000	-0.580000000000
20 H	2.535000000000	3.233000000000	-0.821000000000
21 H	1.138000000000	3.366000000000	0.243000000000
22 H	0.922000000000	2.935000000000	-1.456000000000
23 C	1.664000000000	1.534000000000	2.380000000000
24 H	2.629000000000	1.888000000000	2.764000000000
25 H	1.222000000000	0.904000000000	3.159000000000
26 H	1.022000000000	2.409000000000	2.262000000000
27 C	-2.397000000000	-0.858000000000	0.440000000000
28 C	-2.036000000000	0.317000000000	1.163000000000
29 C	-1.727000000000	1.341000000000	0.218000000000
30 C	-1.838000000000	0.781000000000	-1.087000000000
31 C	-2.255000000000	-0.579000000000	-0.945000000000
32 C	-2.831000000000	-2.176000000000	1.010000000000
33 H	-2.235000000000	-2.995000000000	0.596000000000
34 H	-3.886000000000	-2.371000000000	0.785000000000
35 H	-2.720000000000	-2.200000000000	2.097000000000
36 C	-2.089000000000	0.500000000000	2.655000000000
37 H	-1.906000000000	-0.439000000000	3.186000000000
38 H	-3.071000000000	0.867000000000	2.980000000000
39 H	-1.345000000000	1.225000000000	3.000000000000
40 C	-1.562000000000	2.792000000000	0.558000000000
41 H	-1.137000000000	3.362000000000	-0.268000000000
42 H	-0.927000000000	2.947000000000	1.435000000000
43 H	-2.538000000000	3.239000000000	0.792000000000
44 C	-1.674000000000	1.515000000000	-2.389000000000
45 H	-2.639000000000	1.872000000000	-2.771000000000
46 H	-1.239000000000	0.879000000000	-3.167000000000
47 H	-1.027000000000	2.389000000000	-2.282000000000
48 C	-2.498000000000	-1.569000000000	-2.050000000000
49 H	-3.571000000000	-1.729000000000	-2.212000000000
50 H	-2.051000000000	-2.539000000000	-1.812000000000
51 H	-2.076000000000	-1.227000000000	-2.999000000000
52 F	0.001000000000	-2.390000000000	-0.008000000000

Cp^*_2ScCl

1 Sc	-0.000000000000	-0.355000000000	-0.000000000000
2 Cl	0.000000000000	-2.790000000000	-0.000000000000
3 C	-2.261000000000	-0.431000000000	-0.958000000000
4 C	-2.422000000000	-0.700000000000	0.429000000000
5 C	-2.030000000000	0.465000000000	1.149000000000
6 C	-1.691000000000	1.478000000000	0.205000000000
7 C	-1.803000000000	0.915000000000	-1.099000000000
8 C	-2.568000000000	-1.383000000000	-2.079000000000
9 H	-2.324000000000	-2.411000000000	-1.803000000000
10 H	-1.999000000000	-1.138000000000	-2.982000000000
11 H	-3.631000000000	-1.347000000000	-2.349000000000
12 C	-2.996000000000	-1.950000000000	1.025000000000
13 H	-4.087000000000	-1.865000000000	1.112000000000
14 H	-2.601000000000	-2.140000000000	2.027000000000
15 H	-2.766000000000	-2.825000000000	0.417000000000
16 C	-2.098000000000	0.645000000000	2.641000000000
17 H	-1.382000000000	1.393000000000	2.991000000000
18 H	-1.889000000000	-0.290000000000	3.170000000000
19 H	-3.095000000000	0.976000000000	2.958000000000
20 C	-1.533000000000	2.930000000000	0.545000000000
21 H	-2.513000000000	3.361000000000	0.789000000000
22 H	-1.126000000000	3.507000000000	-0.285000000000
23 H	-0.893000000000	3.093000000000	1.416000000000
24 C	-1.619000000000	1.636000000000	-2.406000000000
25 H	-2.581000000000	1.975000000000	-2.811000000000
26 H	-1.161000000000	0.996000000000	-3.166000000000
27 H	-0.985000000000	2.519000000000	-2.295000000000
28 C	2.422000000000	-0.700000000000	-0.430000000000
29 C	2.029000000000	0.466000000000	-1.149000000000
30 C	1.691000000000	1.478000000000	-0.204000000000
31 C	1.803000000000	0.915000000000	1.100000000000
32 C	2.262000000000	-0.432000000000	0.958000000000
33 C	2.996000000000	-1.949000000000	-1.027000000000
34 H	2.761000000000	-2.826000000000	-0.423000000000
35 H	4.088000000000	-1.866000000000	-1.107000000000
36 H	2.607000000000	-2.135000000000	-2.031000000000
37 C	2.097000000000	0.647000000000	-2.640000000000
38 H	1.887000000000	-0.286000000000	-3.171000000000
39 H	3.095000000000	0.977000000000	-2.958000000000
40 H	1.383000000000	1.398000000000	-2.990000000000
41 C	1.533000000000	2.931000000000	-0.543000000000
42 H	1.125000000000	3.507000000000	0.288000000000
43 H	0.893000000000	3.095000000000	-1.414000000000
44 H	2.513000000000	3.362000000000	-0.785000000000
45 C	1.619000000000	1.634000000000	2.407000000000
46 H	2.580000000000	1.973000000000	2.812000000000
47 H	1.162000000000	0.993000000000	3.167000000000
48 H	0.984000000000	2.516000000000	2.297000000000
49 C	2.569000000000	-1.384000000000	2.078000000000
50 H	3.632000000000	-1.349000000000	2.347000000000
51 H	2.324000000000	-2.413000000000	1.800000000000
52 H	2.000000000000	-1.141000000000	2.981000000000

Cp^*_2ScBr

1 Sc	0.001000000000	-0.091000000000	-0.001000000000
2 C	-2.272000000000	-0.171000000000	-0.952000000000
3 C	-2.428000000000	-0.432000000000	0.437000000000
4 C	-2.025000000000	0.735000000000	1.149000000000
5 C	-1.689000000000	1.742000000000	0.199000000000
6 C	-1.807000000000	1.172000000000	-1.102000000000
7 C	-2.601000000000	-1.116000000000	-2.072000000000
8 H	-2.403000000000	-2.153000000000	-1.790000000000
9 H	-2.011000000000	-0.901000000000	-2.968000000000
10 H	-3.658000000000	-1.037000000000	-2.357000000000
11 C	-3.025000000000	-1.661000000000	1.056000000000
12 H	-4.084000000000	-1.488000000000	1.289000000000
13 H	-2.521000000000	-1.936000000000	1.986000000000
14 H	-2.958000000000	-2.519000000000	0.388000000000
15 C	-2.091000000000	0.916000000000	2.640000000000
16 H	-1.399000000000	1.688000000000	2.986000000000
17 H	-1.851000000000	-0.012000000000	3.170000000000
18 H	-3.097000000000	1.215000000000	2.962000000000
19 C	-1.537000000000	3.198000000000	0.529000000000
20 H	-2.520000000000	3.623000000000	0.770000000000
21 H	-1.135000000000	3.772000000000	-0.305000000000
22 H	-0.898000000000	3.370000000000	1.398000000000
23 C	-1.629000000000	1.884000000000	-2.414000000000
24 H	-2.594000000000	2.213000000000	-2.820000000000
25 H	-1.169000000000	1.240000000000	-3.171000000000
26 H	-1.001000000000	2.772000000000	-2.312000000000
27 C	2.436000000000	-0.419000000000	-0.415000000000
28 C	2.028000000000	0.731000000000	-1.150000000000
29 C	1.676000000000	1.752000000000	-0.220000000000
30 C	1.789000000000	1.205000000000	1.091000000000
31 C	2.265000000000	-0.137000000000	0.968000000000
32 C	3.054000000000	-1.651000000000	-1.006000000000
33 H	2.980000000000	-2.502000000000	-0.328000000000
34 H	4.116000000000	-1.473000000000	-1.220000000000
35 H	2.572000000000	-1.943000000000	-1.942000000000
36 C	2.102000000000	0.889000000000	-2.644000000000
37 H	1.900000000000	-0.055000000000	-3.159000000000
38 H	3.100000000000	1.220000000000	-2.962000000000
39 H	1.385000000000	1.630000000000	-3.009000000000
40 C	1.512000000000	3.199000000000	-0.578000000000
41 H	1.109000000000	3.786000000000	0.247000000000
42 H	0.867000000000	3.349000000000	-1.448000000000
43 H	2.490000000000	3.627000000000	-0.833000000000
44 C	1.599000000000	1.937000000000	2.390000000000
45 H	2.561000000000	2.267000000000	2.803000000000
46 H	1.126000000000	1.308000000000	3.151000000000
47 H	0.977000000000	2.826000000000	2.267000000000
48 C	2.591000000000	-1.062000000000	2.106000000000
49 H	3.647000000000	-0.976000000000	2.393000000000
50 H	2.395000000000	-2.103000000000	1.841000000000
51 H	1.998000000000	-0.830000000000	2.996000000000
52 Br	0.011000000000	-2.695000000000	-0.002000000000

Cp*2ScI

1 Sc	-0.169000000000	0.001000000000	-0.001000000000
2 C	-0.135000000000	2.260000000000	0.994000000000
3 C	0.181000000000	2.452000000000	-0.379000000000
4 C	-0.949000000000	2.049000000000	-1.148000000000
5 C	-1.994000000000	1.689000000000	-0.249000000000
6 C	-1.480000000000	1.783000000000	1.077000000000
7 C	0.748000000000	2.580000000000	2.167000000000
8 H	1.804000000000	2.511000000000	1.901000000000
9 H	0.575000000000	1.892000000000	3.002000000000
10 H	0.554000000000	3.593000000000	2.541000000000
11 C	1.402000000000	3.121000000000	-0.937000000000
12 H	1.177000000000	4.172000000000	-1.160000000000
13 H	1.743000000000	2.650000000000	-1.862000000000
14 H	2.236000000000	3.093000000000	-0.236000000000
15 C	-1.068000000000	2.141000000000	-2.644000000000
16 H	-1.811000000000	1.441000000000	-3.035000000000
17 H	-0.114000000000	1.927000000000	-3.136000000000
18 H	-1.372000000000	3.147000000000	-2.959000000000
19 C	-3.433000000000	1.544000000000	-0.646000000000
20 H	-3.839000000000	2.530000000000	-0.910000000000
21 H	-4.048000000000	1.150000000000	0.162000000000
22 H	-3.570000000000	0.904000000000	-1.521000000000
23 C	-2.243000000000	1.592000000000	2.358000000000
24 H	-2.561000000000	2.556000000000	2.775000000000
25 H	-1.638000000000	1.099000000000	3.126000000000
26 H	-3.142000000000	0.991000000000	2.209000000000
27 C	0.115000000000	-2.441000000000	0.456000000000
28 C	-1.057000000000	-2.007000000000	1.141000000000
29 C	-2.036000000000	-1.655000000000	0.168000000000
30 C	-1.439000000000	-1.786000000000	-1.119000000000
31 C	-0.111000000000	-2.284000000000	-0.939000000000
32 C	1.298000000000	-3.090000000000	1.111000000000
33 H	2.170000000000	-3.096000000000	0.458000000000
34 H	1.057000000000	-4.129000000000	1.372000000000
35 H	1.589000000000	-2.576000000000	2.032000000000
36 C	-1.274000000000	-2.076000000000	2.627000000000
37 H	-0.359000000000	-1.838000000000	3.181000000000
38 H	-1.580000000000	-3.083000000000	2.938000000000
39 H	-2.054000000000	-1.384000000000	2.956000000000
40 C	-3.498000000000	-1.489000000000	0.463000000000
41 H	-4.048000000000	-1.082000000000	-0.385000000000
42 H	-3.686000000000	-0.849000000000	1.329000000000
43 H	-3.936000000000	-2.469000000000	0.693000000000
44 C	-2.112000000000	-1.599000000000	-2.450000000000
45 H	-2.436000000000	-2.561000000000	-2.868000000000
46 H	-1.442000000000	-1.144000000000	-3.187000000000
47 H	-2.997000000000	-0.965000000000	-2.372000000000
48 C	0.832000000000	-2.656000000000	-2.047000000000
49 H	0.607000000000	-3.659000000000	-2.432000000000
50 H	1.869000000000	-2.645000000000	-1.707000000000
51 H	0.759000000000	-1.963000000000	-2.891000000000
52 I	2.671000000000	-0.019000000000	-0.001000000000

$Cp^*_2ScF(THF)$

1 Sc	0.206000000000	-0.009000000000	-0.305000000000
2 C	-0.480000000000	-2.334000000000	0.541000000000
3 C	0.002000000000	-2.492000000000	-0.781000000000
4 C	1.382000000000	-2.150000000000	-0.787000000000
5 C	1.764000000000	-1.817000000000	0.543000000000
6 C	0.599000000000	-1.893000000000	1.363000000000
7 C	0.378000000000	2.077000000000	1.151000000000
8 C	1.705000000000	1.583000000000	1.028000000000
9 C	2.082000000000	1.666000000000	-0.344000000000
10 C	1.000000000000	2.255000000000	-1.057000000000
11 C	-0.051000000000	2.505000000000	-0.142000000000
12 C	-1.837000000000	-2.737000000000	1.040000000000
13 C	-0.767000000000	-2.957000000000	-1.982000000000
14 C	2.273000000000	-2.209000000000	-1.995000000000
15 C	3.183000000000	-1.710000000000	1.020000000000
16 C	0.534000000000	-1.744000000000	2.858000000000
17 C	-0.307000000000	2.300000000000	2.472000000000
18 C	2.604000000000	1.332000000000	2.203000000000
19 C	3.428000000000	1.362000000000	-0.941000000000
20 C	0.980000000000	2.592000000000	-2.517000000000
21 C	-1.341000000000	3.180000000000	-0.510000000000
22 H	-2.632000000000	-2.511000000000	0.324000000000
23 H	-2.088000000000	-2.245000000000	1.984000000000
24 H	-1.876000000000	-3.817000000000	1.230000000000
25 H	-1.808000000000	-3.182000000000	-1.731000000000
26 H	-0.759000000000	-2.193000000000	-2.766000000000
27 H	-0.331000000000	-3.873000000000	-2.399000000000
28 H	1.810000000000	-1.703000000000	-2.849000000000
29 H	3.239000000000	-1.735000000000	-1.805000000000
30 H	2.472000000000	-3.246000000000	-2.297000000000
31 H	3.808000000000	-1.116000000000	0.350000000000
32 H	3.250000000000	-1.271000000000	2.015000000000
33 H	3.634000000000	-2.710000000000	1.075000000000
34 H	0.392000000000	-2.714000000000	3.354000000000
35 H	1.451000000000	-1.310000000000	3.260000000000
36 H	-0.295000000000	-1.101000000000	3.181000000000
37 H	0.330000000000	2.890000000000	3.142000000000
38 H	-1.242000000000	2.854000000000	2.355000000000
39 H	-0.538000000000	1.368000000000	3.004000000000
40 H	-1.162000000000	4.211000000000	-0.841000000000
41 H	-1.850000000000	2.668000000000	-1.334000000000
42 H	-2.035000000000	3.231000000000	0.332000000000
43 H	0.044000000000	2.276000000000	-2.985000000000
44 H	1.099000000000	3.672000000000	-2.675000000000
45 H	1.791000000000	2.089000000000	-3.050000000000
46 H	3.359000000000	0.682000000000	-1.798000000000
47 H	3.914000000000	2.278000000000	-1.300000000000
48 H	4.100000000000	0.906000000000	-0.211000000000
49 H	3.564000000000	0.911000000000	1.904000000000
50 H	2.158000000000	0.661000000000	2.942000000000
51 H	2.814000000000	2.278000000000	2.721000000000
52 F	-0.254000000000	-0.001000000000	-2.180000000000
53 O	-2.040000000000	0.184000000000	-0.010000000000
54 C	-2.800000000000	0.465000000000	1.188000000000
55 C	-2.934000000000	-0.026000000000	-1.145000000000
56 C	-4.239000000000	0.089000000000	0.849000000000
57 H	-2.368000000000	-0.111000000000	2.008000000000
58 H	-2.708000000000	1.528000000000	1.414000000000
59 C	-4.304000000000	0.421000000000	-0.649000000000
60 H	-2.533000000000	0.537000000000	-1.985000000000
61 H	-2.910000000000	-1.090000000000	-1.397000000000
62 H	-4.961000000000	0.648000000000	1.450000000000
63 H	-4.406000000000	-0.979000000000	1.014000000000
64 H	-4.431000000000	1.499000000000	-0.794000000000

65 H	-5.116000000000	-0.092000000000	-1.170000000000

$Cp^*_2ScCl(THF)$

1 Sc	-0.218000000000	0.012000000000	-0.235000000000
2 C	0.566000000000	2.277000000000	0.694000000000
3 C	0.110000000000	2.525000000000	-0.624000000000
4 C	-1.286000000000	2.246000000000	-0.661000000000
5 C	-1.697000000000	1.862000000000	0.643000000000
6 C	-0.540000000000	1.840000000000	1.480000000000
7 C	-0.470000000000	-1.993000000000	1.299000000000
8 C	-1.783000000000	-1.480000000000	1.090000000000
9 C	-2.106000000000	-1.644000000000	-0.287000000000
10 C	-1.019000000000	-2.318000000000	-0.912000000000
11 C	-0.009000000000	-2.528000000000	0.058000000000
12 C	1.924000000000	2.627000000000	1.227000000000
13 C	0.906000000000	3.122000000000	-1.745000000000
14 C	-2.193000000000	2.463000000000	-1.837000000000
15 C	-3.131000000000	1.820000000000	1.085000000000
16 C	-0.504000000000	1.662000000000	2.972000000000
17 C	0.143000000000	-2.171000000000	2.662000000000
18 C	-2.745000000000	-1.194000000000	2.205000000000
19 C	-3.407000000000	-1.327000000000	-0.968000000000
20 C	-1.020000000000	-2.871000000000	-2.304000000000
21 C	1.256000000000	-3.293000000000	-0.205000000000
22 H	2.721000000000	2.425000000000	0.506000000000
23 H	2.158000000000	2.088000000000	2.149000000000
24 H	1.978000000000	3.697000000000	1.467000000000
25 H	1.981000000000	3.071000000000	-1.549000000000
26 H	0.714000000000	2.605000000000	-2.688000000000
27 H	0.653000000000	4.182000000000	-1.878000000000
28 H	-1.670000000000	2.275000000000	-2.776000000000
29 H	-3.060000000000	1.795000000000	-1.803000000000
30 H	-2.576000000000	3.492000000000	-1.858000000000
31 H	-3.755000000000	1.201000000000	0.437000000000
32 H	-3.238000000000	1.455000000000	2.106000000000
33 H	-3.553000000000	2.833000000000	1.056000000000
34 H	-0.388000000000	2.626000000000	3.484000000000
35 H	-1.421000000000	1.207000000000	3.349000000000
36 H	0.330000000000	1.030000000000	3.299000000000
37 H	-0.520000000000	-2.761000000000	3.307000000000
38 H	1.095000000000	-2.705000000000	2.613000000000
39 H	0.321000000000	-1.224000000000	3.183000000000
40 H	1.032000000000	-4.251000000000	-0.686000000000
41 H	1.940000000000	-2.755000000000	-0.871000000000
42 H	1.796000000000	-3.520000000000	0.718000000000
43 H	-0.015000000000	-2.906000000000	-2.728000000000
44 H	-1.428000000000	-3.892000000000	-2.303000000000
45 H	-1.628000000000	-2.264000000000	-2.977000000000
46 H	-3.249000000000	-0.780000000000	-1.904000000000
47 H	-3.956000000000	-2.243000000000	-1.220000000000
48 H	-4.062000000000	-0.723000000000	-0.336000000000
49 H	-3.661000000000	-0.722000000000	1.851000000000
50 H	-2.317000000000	-0.563000000000	2.986000000000
51 H	-3.034000000000	-2.139000000000	2.686000000000
52 Cl	0.150000000000	0.014000000000	-2.682000000000
53 O	2.028000000000	-0.271000000000	0.011000000000
54 C	2.721000000000	-0.595000000000	1.242000000000
55 C	2.991000000000	-0.033000000000	-1.063000000000
56 C	4.175000000000	-0.205000000000	1.004000000000
57 H	2.240000000000	-0.055000000000	2.058000000000
58 H	2.621000000000	-1.667000000000	1.419000000000
59 C	4.333000000000	-0.484000000000	-0.497000000000
60 H	2.649000000000	-0.586000000000	-1.937000000000
61 H	2.971000000000	1.034000000000	-1.298000000000
62 H	4.861000000000	-0.786000000000	1.627000000000
63 H	4.330000000000	0.856000000000	1.218000000000

64 H	4.481000000000	-1.555000000000	-0.670000000000
65 H	5.168000000000	0.054000000000	-0.950000000000

$Cp^*_2ScBr(THF)$

1 Sc	-0.227000000000	0.014000000000	-0.038000000000
2 C	0.530000000000	2.263000000000	0.927000000000
3 C	0.038000000000	2.539000000000	-0.371000000000
4 C	-1.355000000000	2.241000000000	-0.383000000000
5 C	-1.726000000000	1.815000000000	0.921000000000
6 C	-0.549000000000	1.788000000000	1.729000000000
7 C	-0.478000000000	-2.035000000000	1.446000000000
8 C	-1.793000000000	-1.525000000000	1.248000000000
9 C	-2.112000000000	-1.652000000000	-0.133000000000
10 C	-1.021000000000	-2.306000000000	-0.774000000000
11 C	-0.009000000000	-2.530000000000	0.192000000000
12 C	1.895000000000	2.639000000000	1.422000000000
13 C	0.809000000000	3.205000000000	-1.471000000000
14 C	-2.303000000000	2.476000000000	-1.523000000000
15 C	-3.147000000000	1.751000000000	1.400000000000
16 C	-0.478000000000	1.563000000000	3.213000000000
17 C	0.122000000000	-2.259000000000	2.808000000000
18 C	-2.760000000000	-1.285000000000	2.369000000000
19 C	-3.416000000000	-1.327000000000	-0.805000000000
20 C	-1.036000000000	-2.864000000000	-2.164000000000
21 C	1.266000000000	-3.270000000000	-0.093000000000
22 H	2.675000000000	2.431000000000	0.686000000000
23 H	2.157000000000	2.127000000000	2.351000000000
24 H	1.940000000000	3.716000000000	1.632000000000
25 H	1.844000000000	2.854000000000	-1.520000000000
26 H	0.361000000000	3.014000000000	-2.446000000000
27 H	0.839000000000	4.292000000000	-1.313000000000
28 H	-1.816000000000	2.299000000000	-2.485000000000
29 H	-3.170000000000	1.812000000000	-1.466000000000
30 H	-2.682000000000	3.507000000000	-1.517000000000
31 H	-3.788000000000	1.151000000000	0.749000000000
32 H	-3.225000000000	1.353000000000	2.410000000000
33 H	-3.572000000000	2.763000000000	1.415000000000
34 H	-0.397000000000	2.514000000000	3.756000000000
35 H	-1.366000000000	1.053000000000	3.589000000000
36 H	0.389000000000	0.959000000000	3.504000000000
37 H	-0.559000000000	-2.852000000000	3.431000000000
38 H	1.062000000000	-2.814000000000	2.752000000000
39 H	0.316000000000	-1.331000000000	3.356000000000
40 H	1.053000000000	-4.259000000000	-0.514000000000
41 H	1.895000000000	-2.743000000000	-0.819000000000
42 H	1.859000000000	-3.430000000000	0.812000000000
43 H	-0.034000000000	-2.910000000000	-2.597000000000
44 H	-1.449000000000	-3.882000000000	-2.151000000000
45 H	-1.647000000000	-2.260000000000	-2.837000000000
46 H	-3.260000000000	-0.793000000000	-1.748000000000
47 H	-3.978000000000	-2.240000000000	-1.042000000000
48 H	-4.057000000000	-0.708000000000	-0.174000000000
49 H	-3.682000000000	-0.816000000000	2.029000000000
50 H	-2.342000000000	-0.673000000000	3.172000000000
51 H	-3.035000000000	-2.249000000000	2.820000000000
52 Br	0.207000000000	0.094000000000	-2.654000000000
53 O	2.020000000000	-0.271000000000	0.268000000000
54 C	2.661000000000	-0.572000000000	1.533000000000
55 C	3.031000000000	-0.071000000000	-0.770000000000
56 C	4.123000000000	-0.182000000000	1.352000000000
57 H	2.142000000000	-0.018000000000	2.316000000000
58 H	2.557000000000	-1.640000000000	1.724000000000
59 C	4.348000000000	-0.500000000000	-0.132000000000
60 H	2.736000000000	-0.654000000000	-1.640000000000
61 H	3.020000000000	0.987000000000	-1.045000000000
62 H	4.781000000000	-0.744000000000	2.020000000000

63 H	4.265000000000	0.885000000000	1.544000000000
64 H	4.506000000000	-1.575000000000	-0.270000000000
65 H	5.201000000000	0.029000000000	-0.563000000000

$Cp^*_2ScI(THF)$

1 Sc	0.274000000000	0.126000000000	0.025000000000
2 C	-0.317000000000	1.083000000000	2.332000000000
3 C	-0.124000000000	-0.307000000000	2.530000000000
4 C	1.241000000000	-0.602000000000	2.246000000000
5 C	1.893000000000	0.611000000000	1.903000000000
6 C	0.919000000000	1.657000000000	1.919000000000
7 C	0.882000000000	1.711000000000	-1.870000000000
8 C	2.111000000000	1.173000000000	-1.390000000000
9 C	2.116000000000	-0.224000000000	-1.658000000000
10 C	0.924000000000	-0.535000000000	-2.373000000000
11 C	0.158000000000	0.651000000000	-2.494000000000
12 C	-1.551000000000	1.836000000000	2.730000000000
13 C	-1.126000000000	-1.236000000000	3.149000000000
14 C	1.928000000000	-1.922000000000	2.444000000000
15 C	3.386000000000	0.768000000000	1.880000000000
16 C	1.181000000000	3.132000000000	1.806000000000
17 C	0.606000000000	3.188000000000	-1.958000000000
18 C	3.309000000000	2.016000000000	-1.063000000000
19 C	3.232000000000	-1.198000000000	-1.405000000000
20 C	0.665000000000	-1.809000000000	-3.119000000000
21 C	-1.123000000000	0.737000000000	-3.273000000000
22 H	-2.468000000000	1.307000000000	2.457000000000
23 H	-1.590000000000	2.835000000000	2.291000000000
24 H	-1.578000000000	1.970000000000	3.820000000000
25 H	-2.144000000000	-1.031000000000	2.807000000000
26 H	-0.912000000000	-2.278000000000	2.914000000000
27 H	-1.121000000000	-1.123000000000	4.242000000000
28 H	1.241000000000	-2.756000000000	2.295000000000
29 H	2.757000000000	-2.054000000000	1.742000000000
30 H	2.345000000000	-1.998000000000	3.458000000000
31 H	3.879000000000	0.037000000000	1.234000000000
32 H	3.692000000000	1.763000000000	1.562000000000
33 H	3.783000000000	0.613000000000	2.892000000000
34 H	1.293000000000	3.592000000000	2.797000000000
35 H	2.095000000000	3.344000000000	1.249000000000
36 H	0.365000000000	3.662000000000	1.303000000000
37 H	1.417000000000	3.695000000000	-2.496000000000
38 H	-0.316000000000	3.398000000000	-2.505000000000
39 H	0.529000000000	3.675000000000	-0.980000000000
40 H	-0.988000000000	0.320000000000	-4.277000000000
41 H	-1.935000000000	0.173000000000	-2.801000000000
42 H	-1.458000000000	1.769000000000	-3.399000000000
43 H	-0.401000000000	-2.030000000000	-3.201000000000
44 H	1.075000000000	-1.726000000000	-4.136000000000
45 H	1.134000000000	-2.667000000000	-2.636000000000
46 H	2.857000000000	-2.136000000000	-0.982000000000
47 H	3.757000000000	-1.451000000000	-2.335000000000
48 H	3.975000000000	-0.794000000000	-0.714000000000
49 H	4.128000000000	1.431000000000	-0.647000000000
50 H	3.088000000000	2.832000000000	-0.372000000000
51 H	3.681000000000	2.479000000000	-1.987000000000
52 I	-0.725000000000	-2.603000000000	-0.123000000000
53 O	-1.870000000000	0.892000000000	-0.249000000000
54 C	-2.206000000000	2.286000000000	-0.465000000000
55 C	-3.088000000000	0.097000000000	-0.112000000000
56 C	-3.682000000000	2.412000000000	-0.106000000000
57 H	-1.540000000000	2.893000000000	0.149000000000
58 H	-2.032000000000	2.520000000000	-1.515000000000
59 C	-4.221000000000	1.035000000000	-0.514000000000
60 H	-2.977000000000	-0.784000000000	-0.741000000000
61 H	-3.160000000000	-0.228000000000	0.929000000000

62 H	-4.160000000000	3.239000000000	-0.637000000000
63 H	-3.807000000000	2.574000000000	0.968000000000
64 H	-4.383000000000	0.995000000000	-1.596000000000
65 H	-5.160000000000	0.774000000000	-0.020000000000