

Supplementary information

Carborane-containing stereoregular cyclic phenylsiloxanes: synthesis, structure and properties

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Table of contents

Synthesis data	2
NMR spectra.....	3
¹ H NMR spectra of initial hydride macrocycles.....	3
NMR spectra of carborane-containing phenylcyclsiloxanes.....	8
IR spectra	28
GPC data.....	33
TGA data	34
Mass spectra	37

Synthesis data

Table S1.

compound	hydride cycle			carborane		toluene	catalyst	reaction time, h	yield after prep. purification	
	Ph _x SiH	gram	mmol	gram	mmol	mL	μL		gram	%
cycle 4	Ph ₄ SiH	0.96	1.2	1.1	5.8	20	10	8	1.51	82
cycle 5	Ph ₅ SiH	0.69	0.7	0.8	4.2	15	10	10	1.05	79
cycle 6	Ph ₆ SiH	0.94	0.8	1.07	5.7	20	10	12	1.45	80
cycle 8	Ph ₈ SiH	1.00	0.6	1.13	6.1	21	10	16	1.41	75
cycle 12	Ph ₁₂ SiH	0.92	0.4	1.3	7.0	22	10	24	1.28	71

NMR spectra

^1H NMR spectra of initial hydride macrocycles

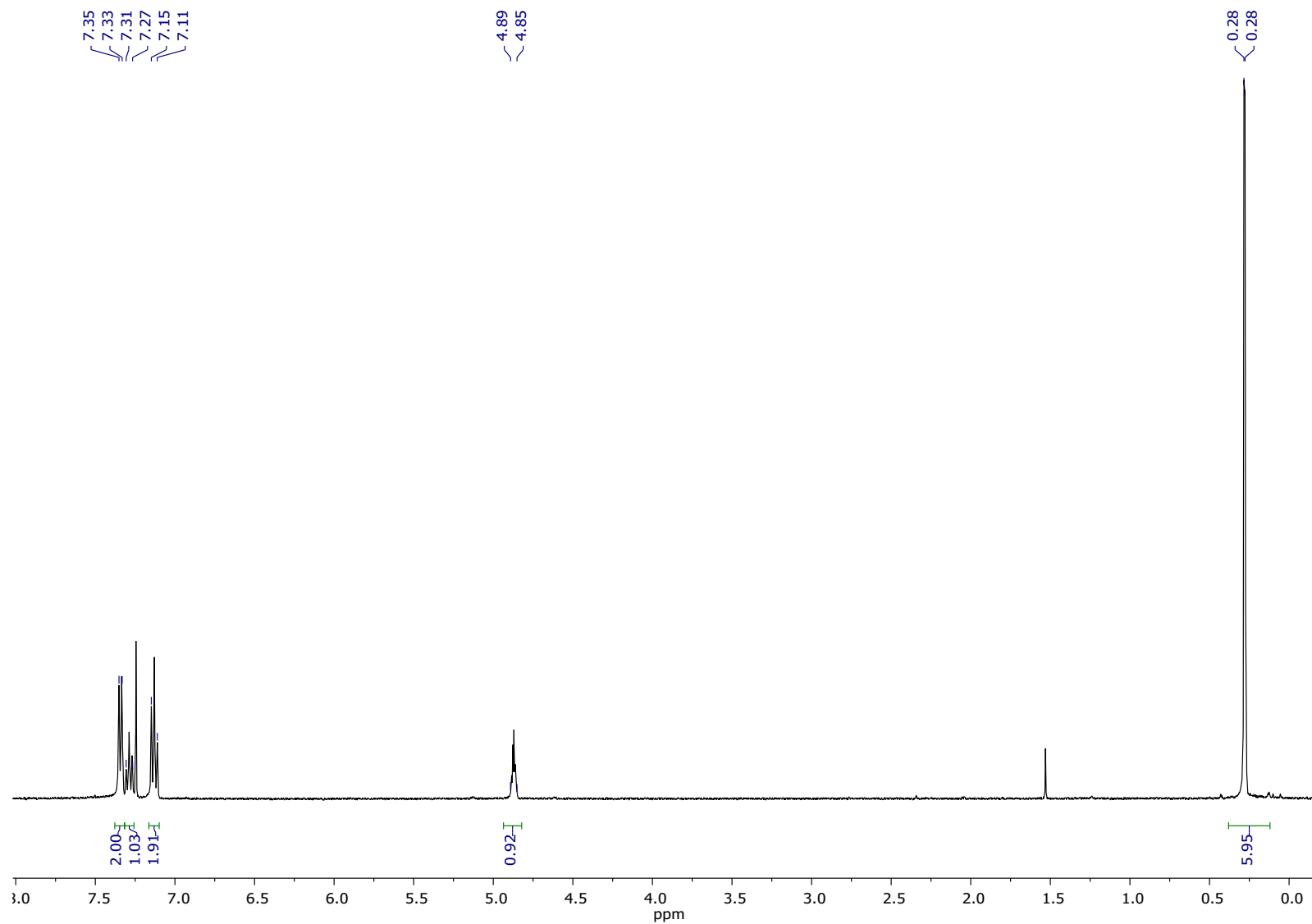


Fig S1. ^1H NMR (CDCl₃) spectrum of *cis*-tetra[(dimethylsiloxy)phenyl]cyclotetrasiloxane (*cis*-[(Ph)(OSiMe₂H)O]₄)

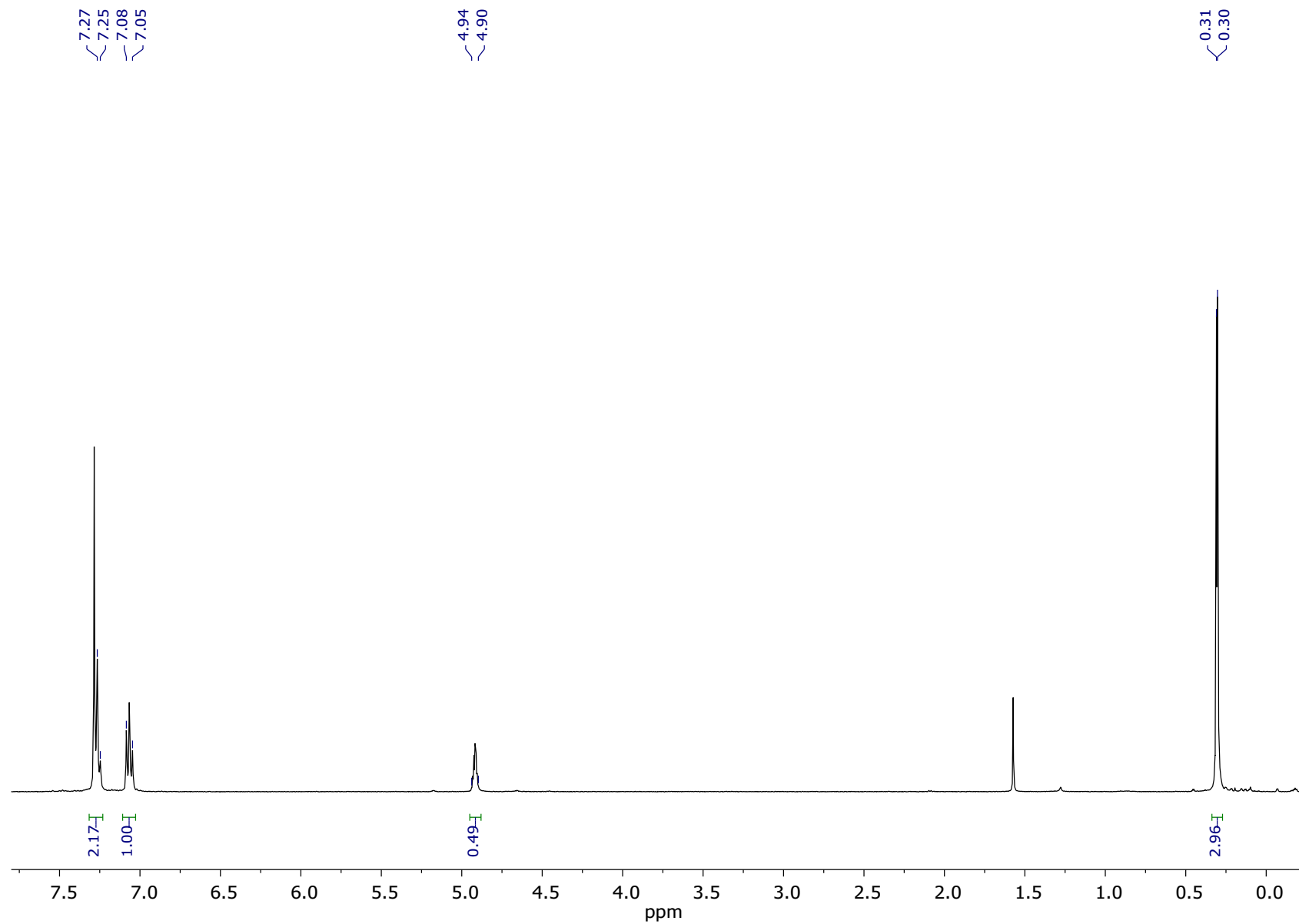


Fig S2. ^1H NMR (CDCl_3) spectrum of *cis*-penta[(dimethylsiloxy)phenyl]cyclopentasiloxane (*cis*-[(Ph)(OSiMe₂H)O]₅)

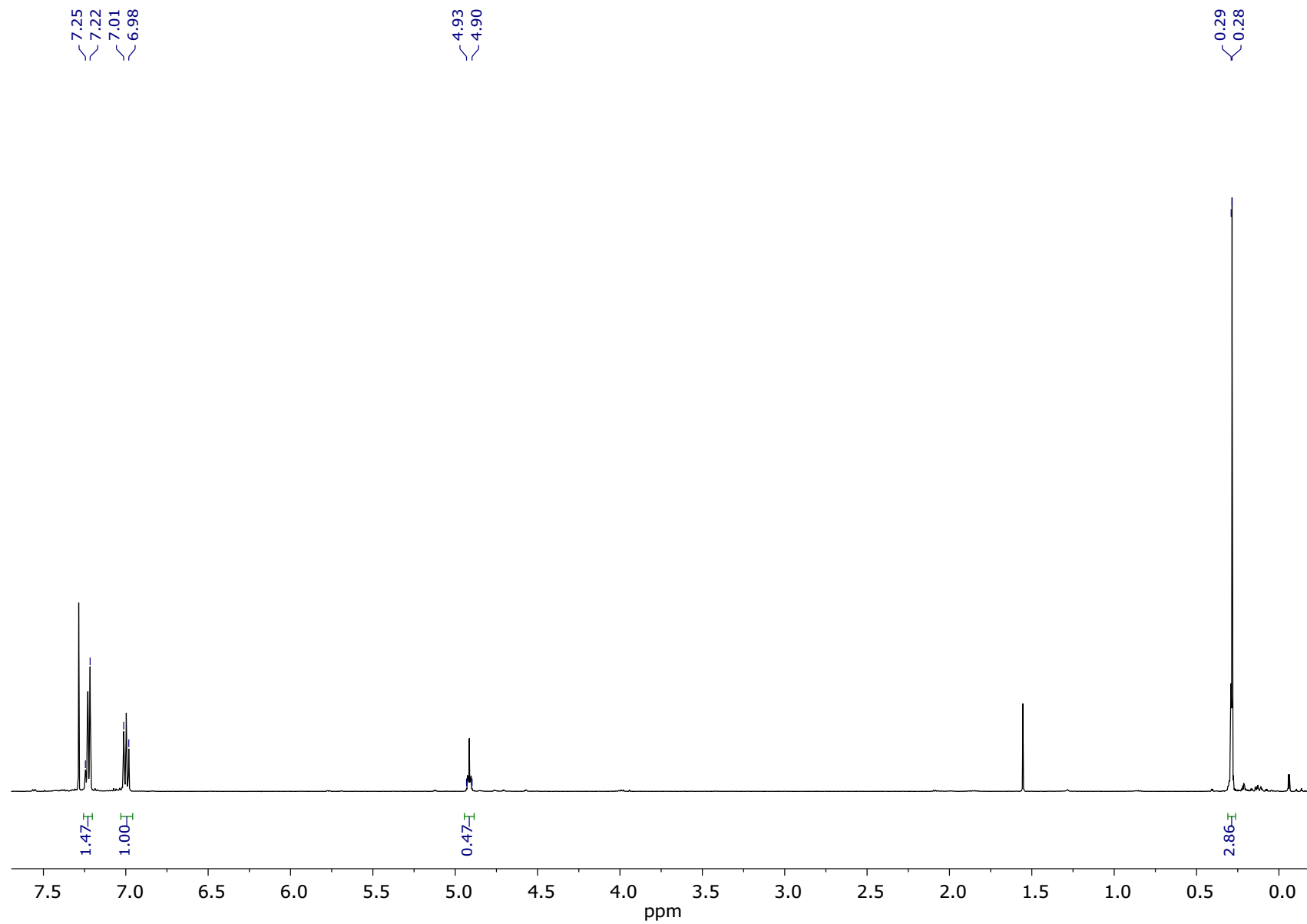


Fig S3. ^1H NMR (CDCl_3) spectrum of *cis*-hexa[(dimethylsiloxy)phenyl]cyclohexasiloxane (*cis*-[(Ph)(OSiMe₂H)O]₆)

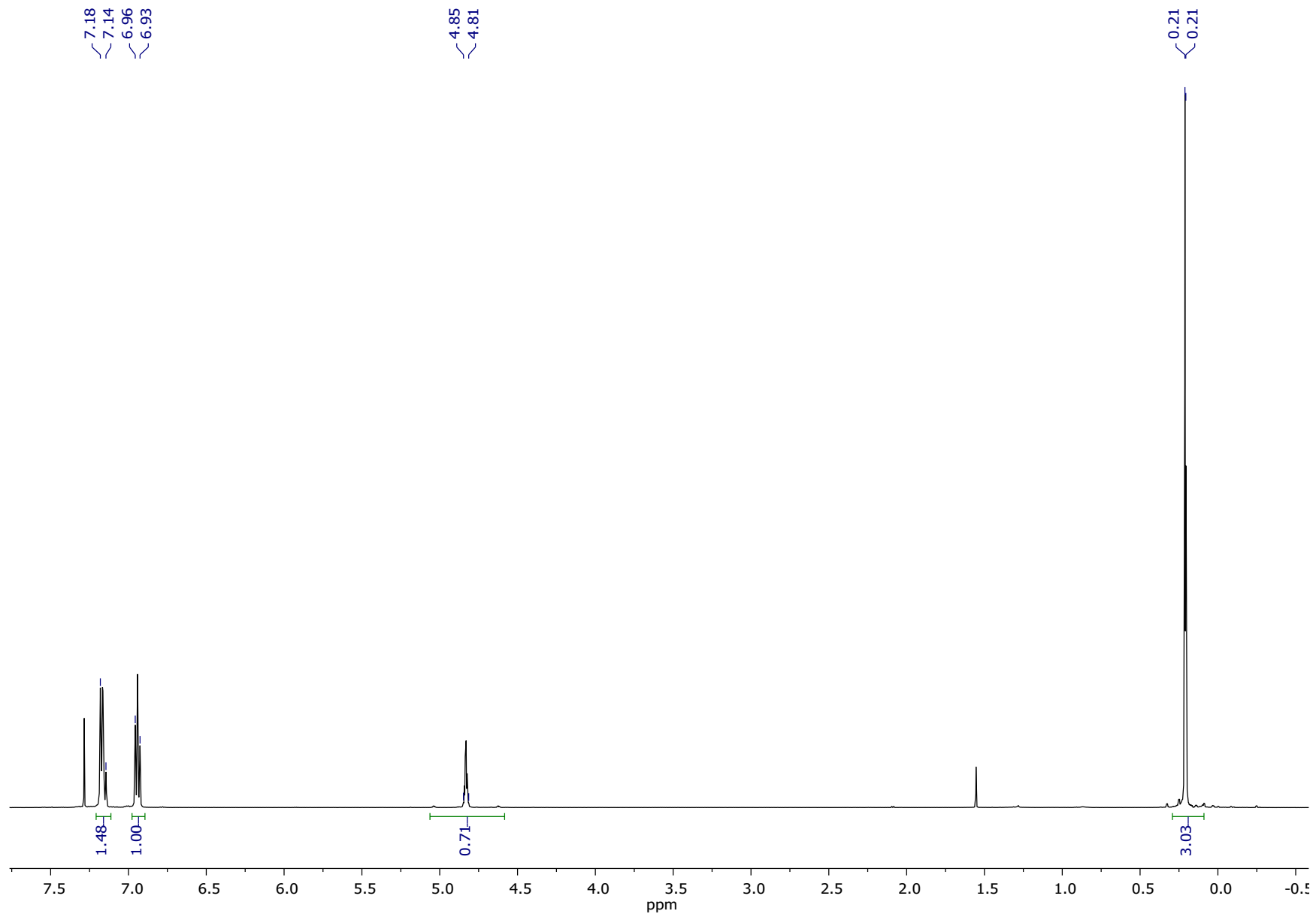


Fig S4. ^1H NMR (CDCl_3) spectrum of *cis*-octa[(dimethylsiloxy)phenyl]cyclooctasiloxane (*cis*-[(Ph)(OSiMe₂H)O]₈)

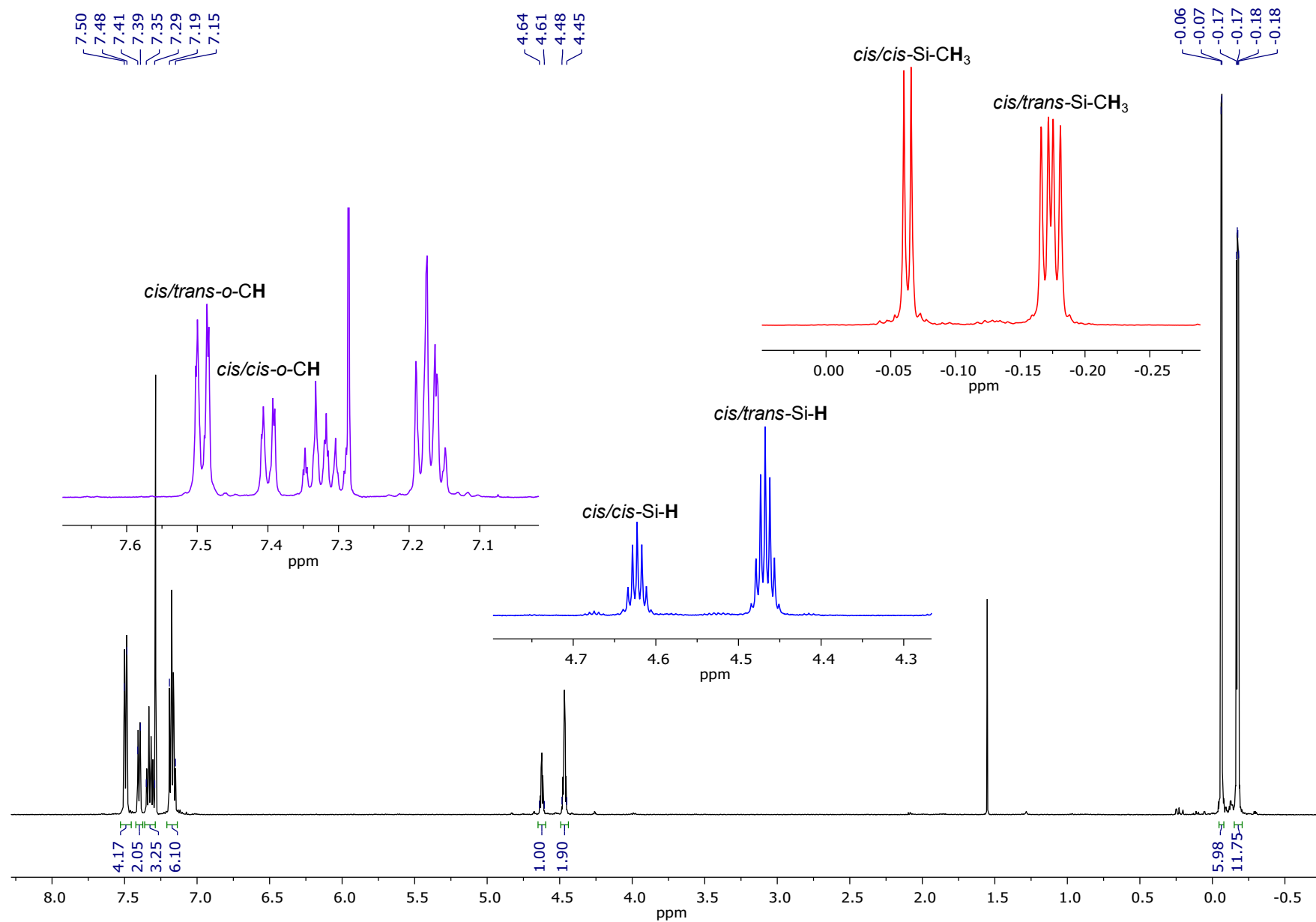


Fig S5. ^1H NMR (CDCl_3) spectrum of tris-*cis*-tris-*trans*-dodeca[(dimethylsiloxy)phenyl]cyclododecasiloxane (tris-*cis*-tris-*trans*-[(Ph)(OSiMe₂H)O]₁₂)

NMR spectra of carborane-containing phenylcyclsiloxanes

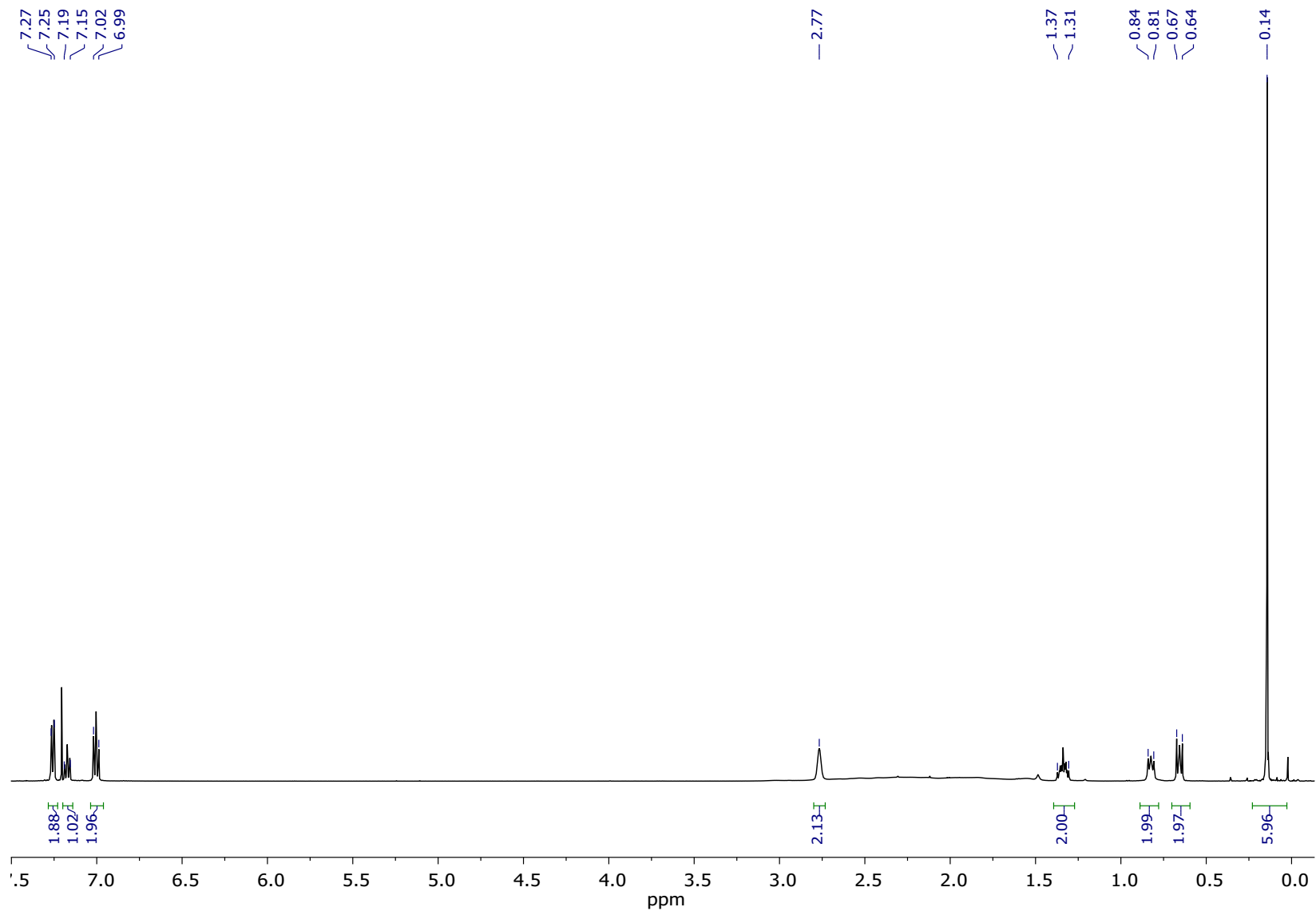


Fig S6. ¹H NMR (CDCl₃) spectrum of *cis*-tetra[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclotetrasiloxane (cycle 4)

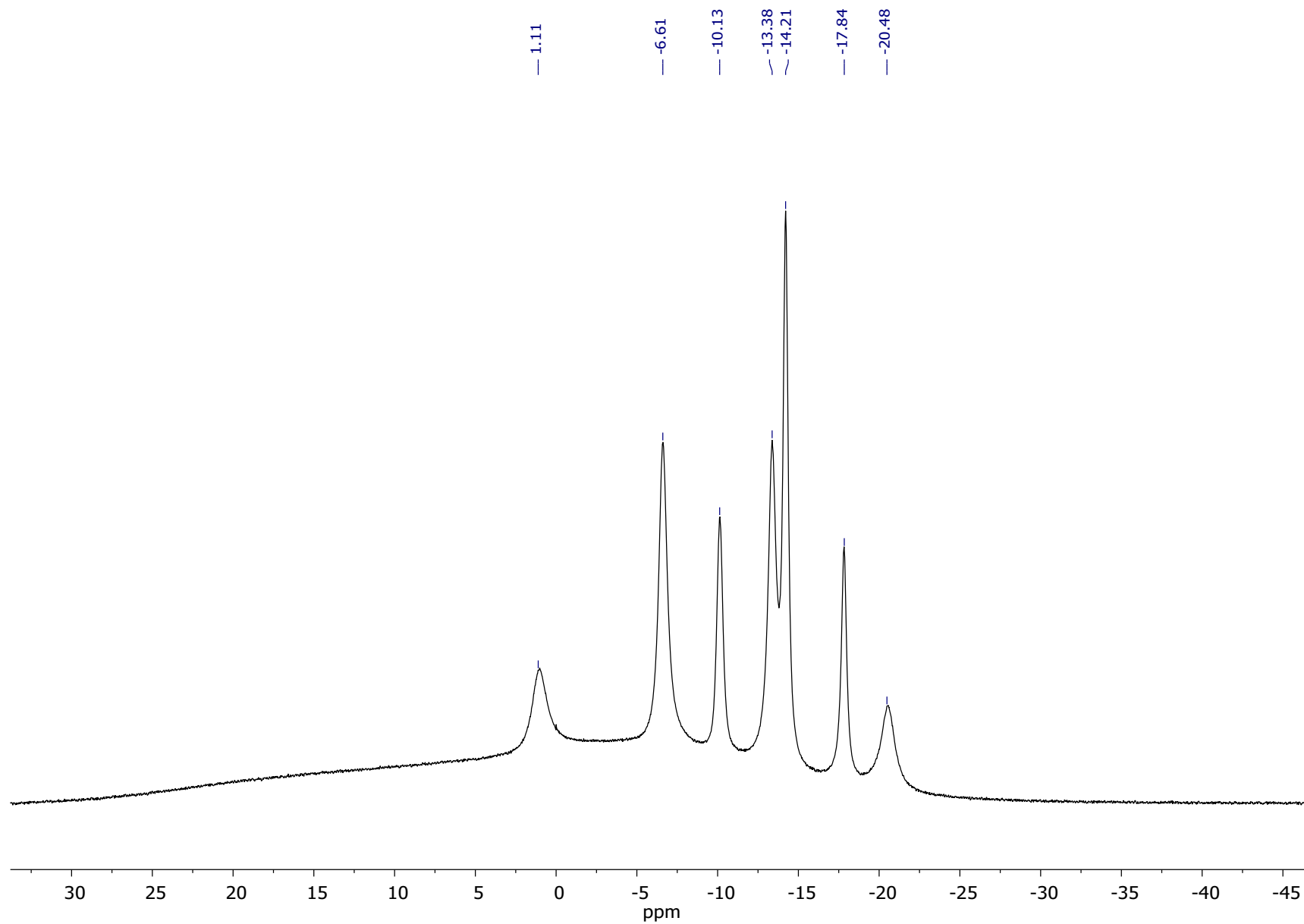


Fig S7. ^{11}B NMR (CDCl_3) spectrum of *cis*-tetra[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclotetrasiloxane (cycle 4)

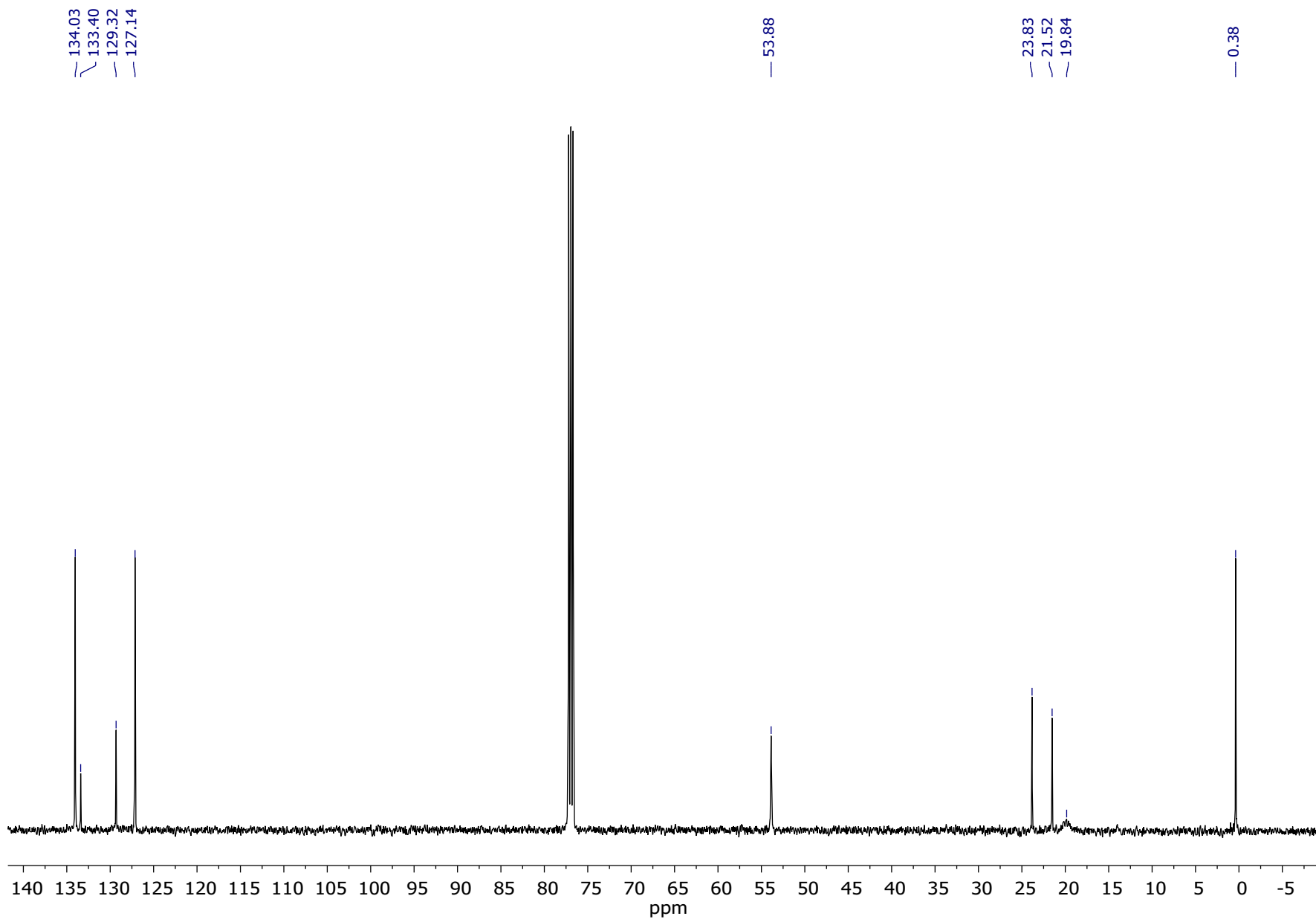


Fig S8. ^{13}C NMR (CDCl_3) spectrum of *cis*-tetra[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclotetrasiloxane (cycle 4)

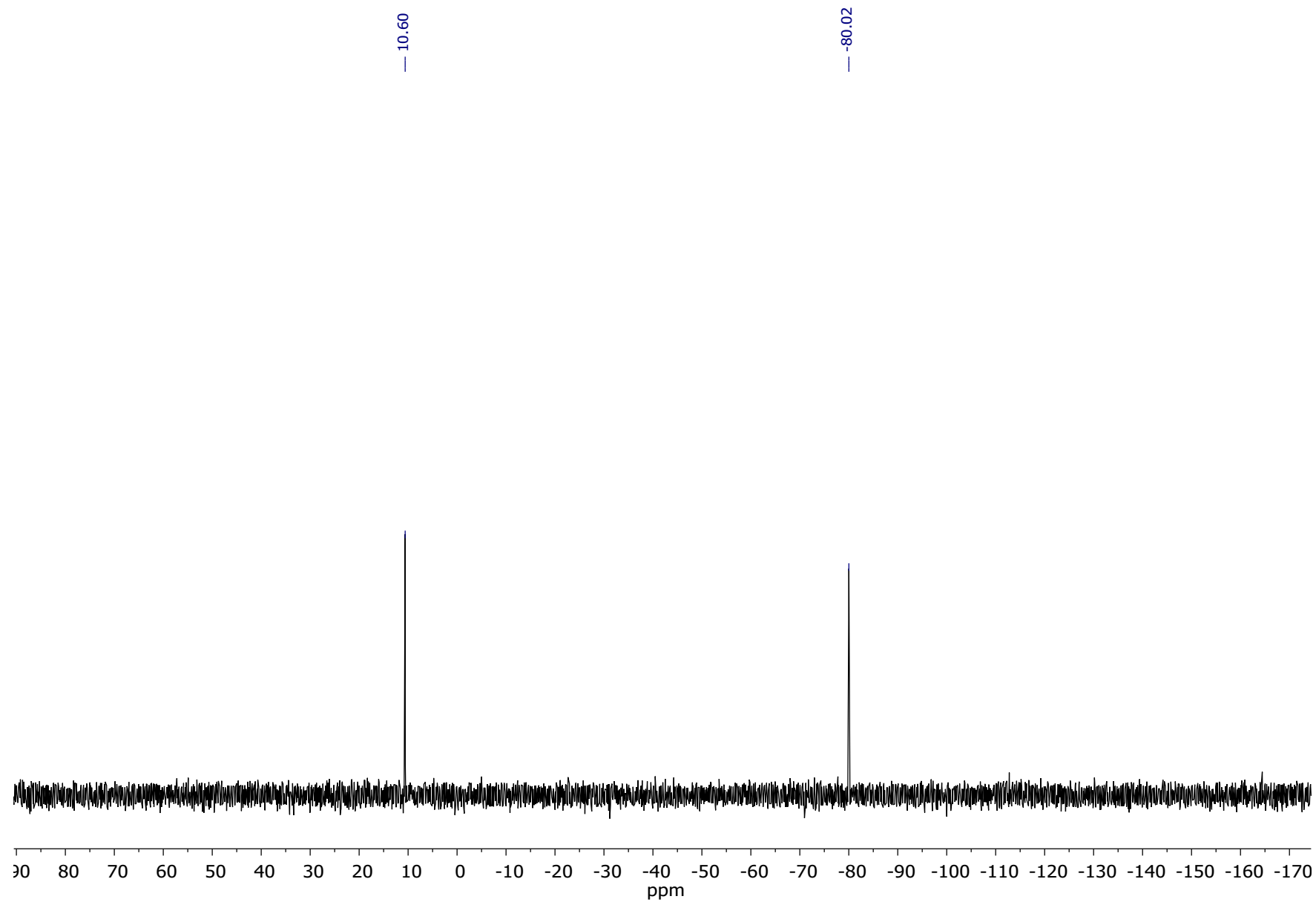


Fig S9. ^{29}Si NMR (CDCl_3) spectrum of *cis*-tetra[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclotetrasiloxane (cycle 4)

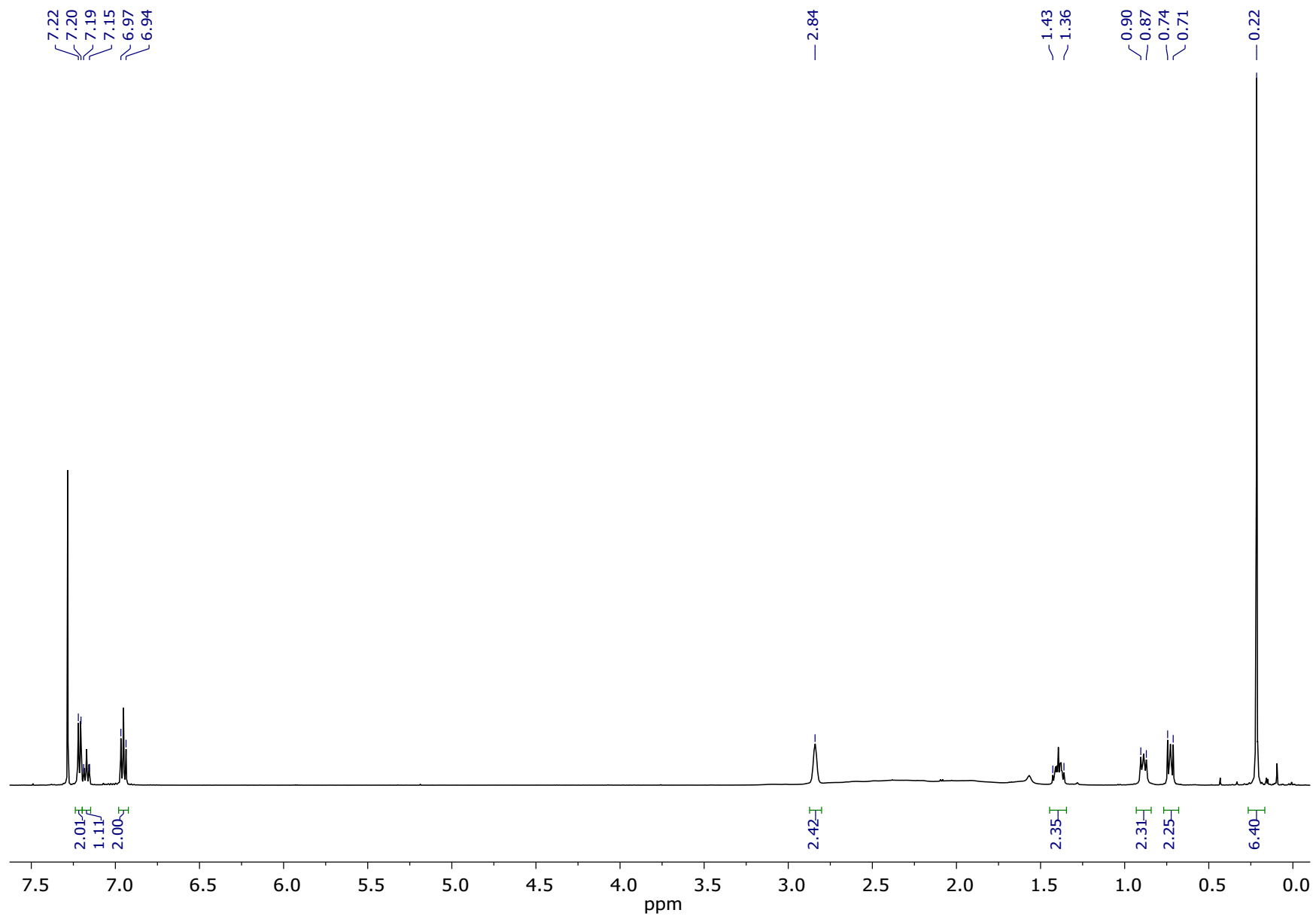


Fig S10. ^1H NMR (CDCl_3) spectrum of *cis*-penta[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclopentasiloxane (cycle 5)

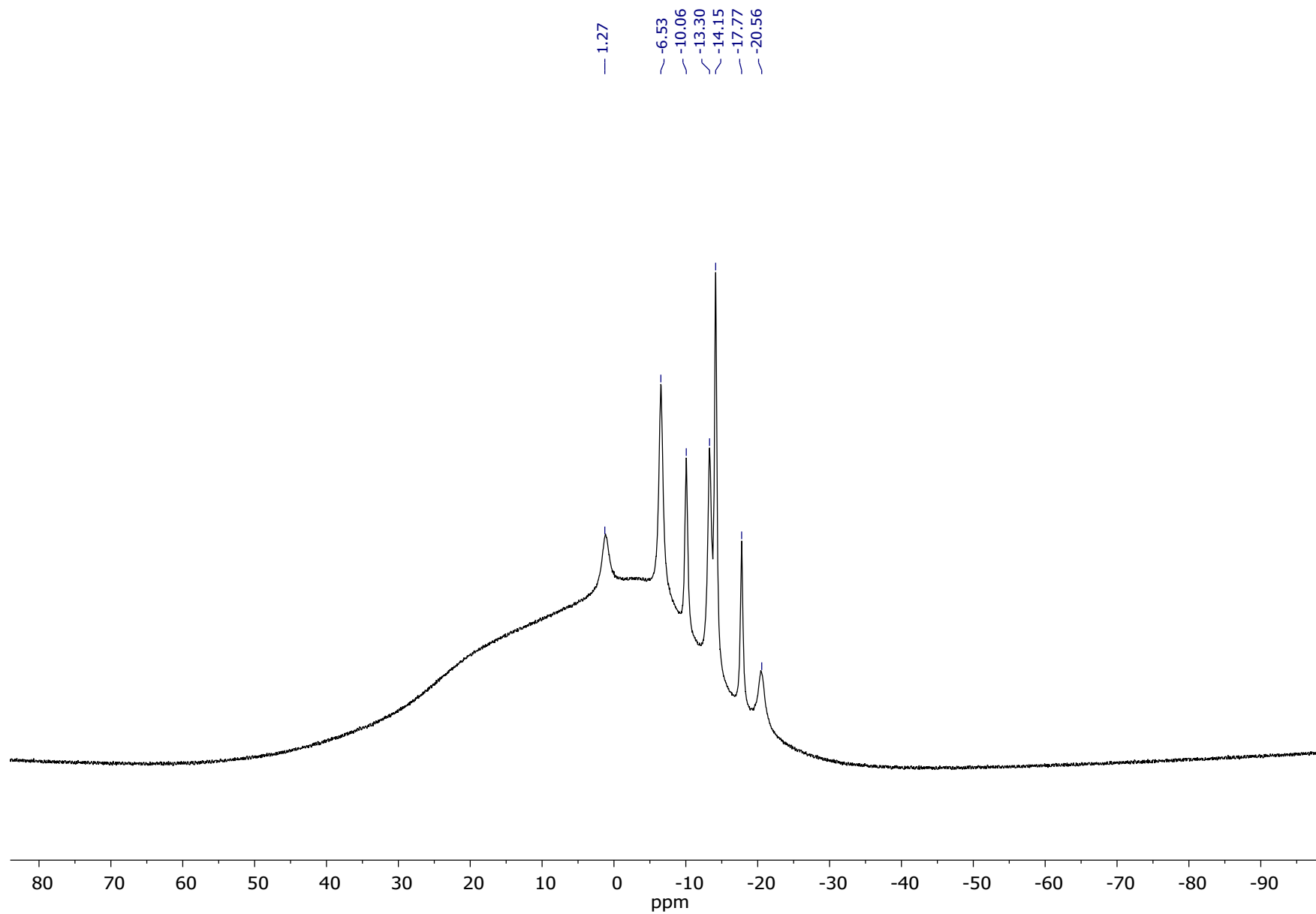


Fig S11. ^{11}B NMR (CDCl_3) spectrum of *cis*-penta[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclopentasiloxane (cycle 5)

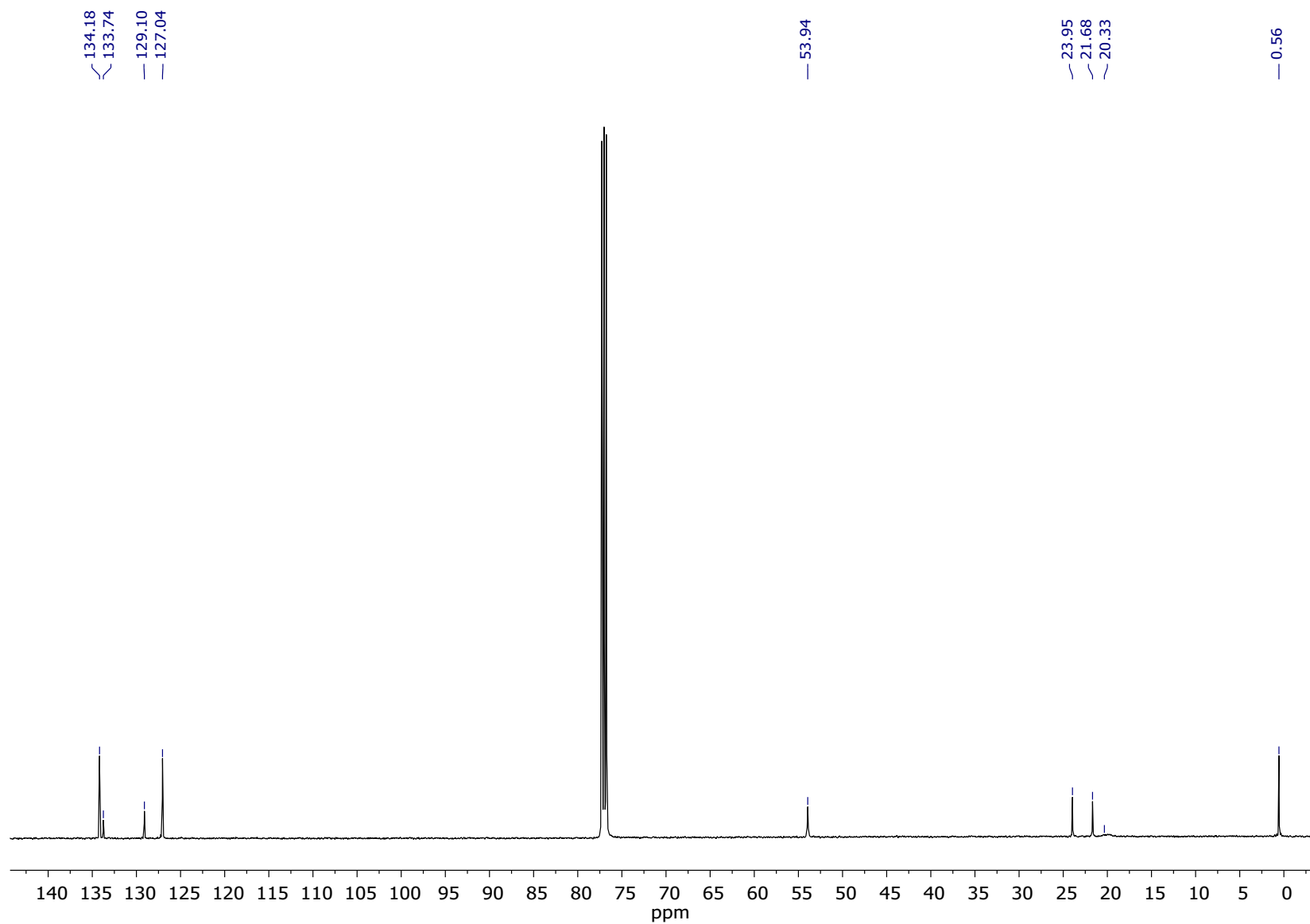


Fig S12. ^{13}C NMR (CDCl_3) spectrum of *cis*-penta[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclopentasiloxane (cycle 5)

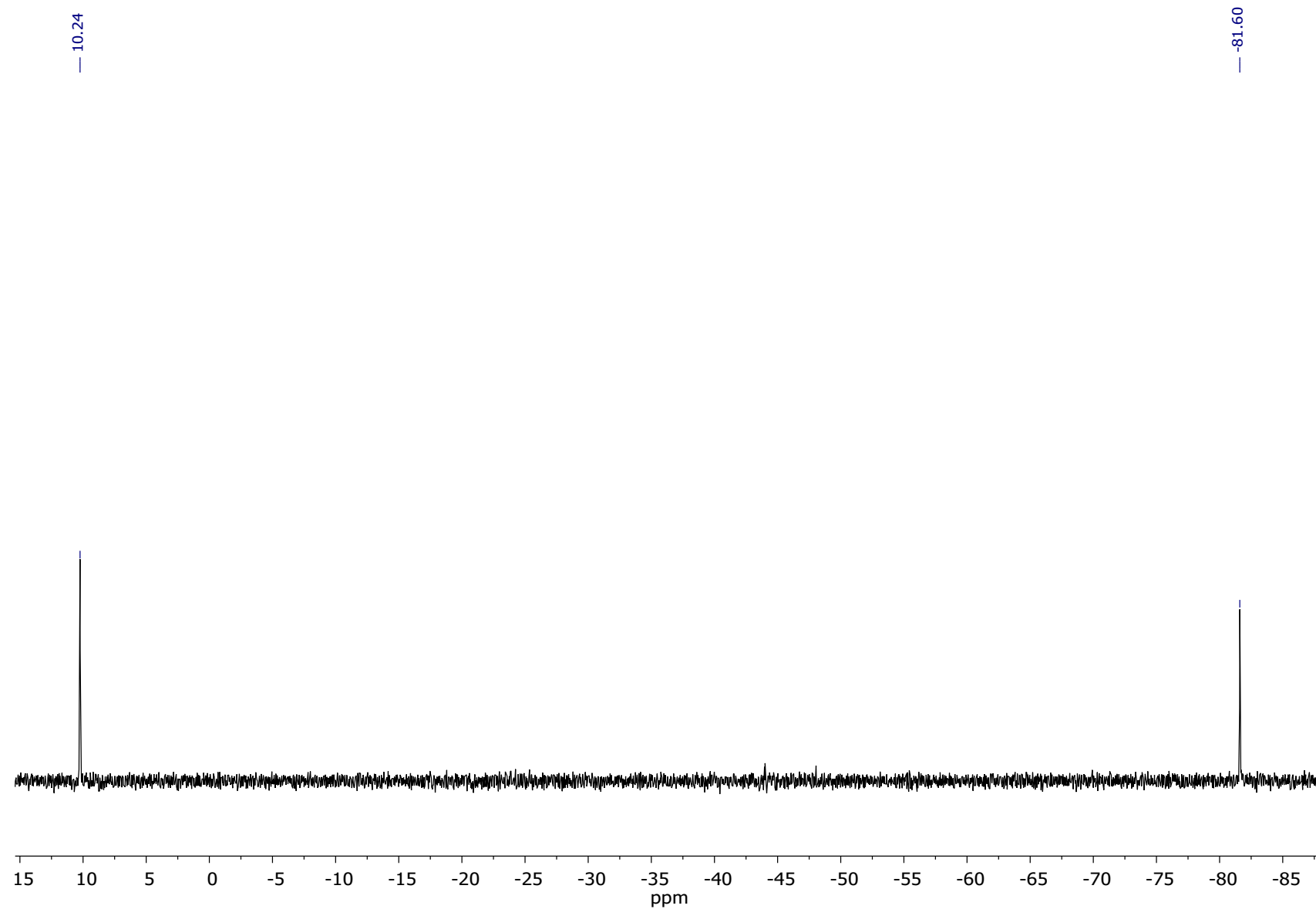


Fig S13. ^{29}Si NMR (CDCl_3) spectrum of *cis*-penta[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclopentasiloxane (cycle 5)

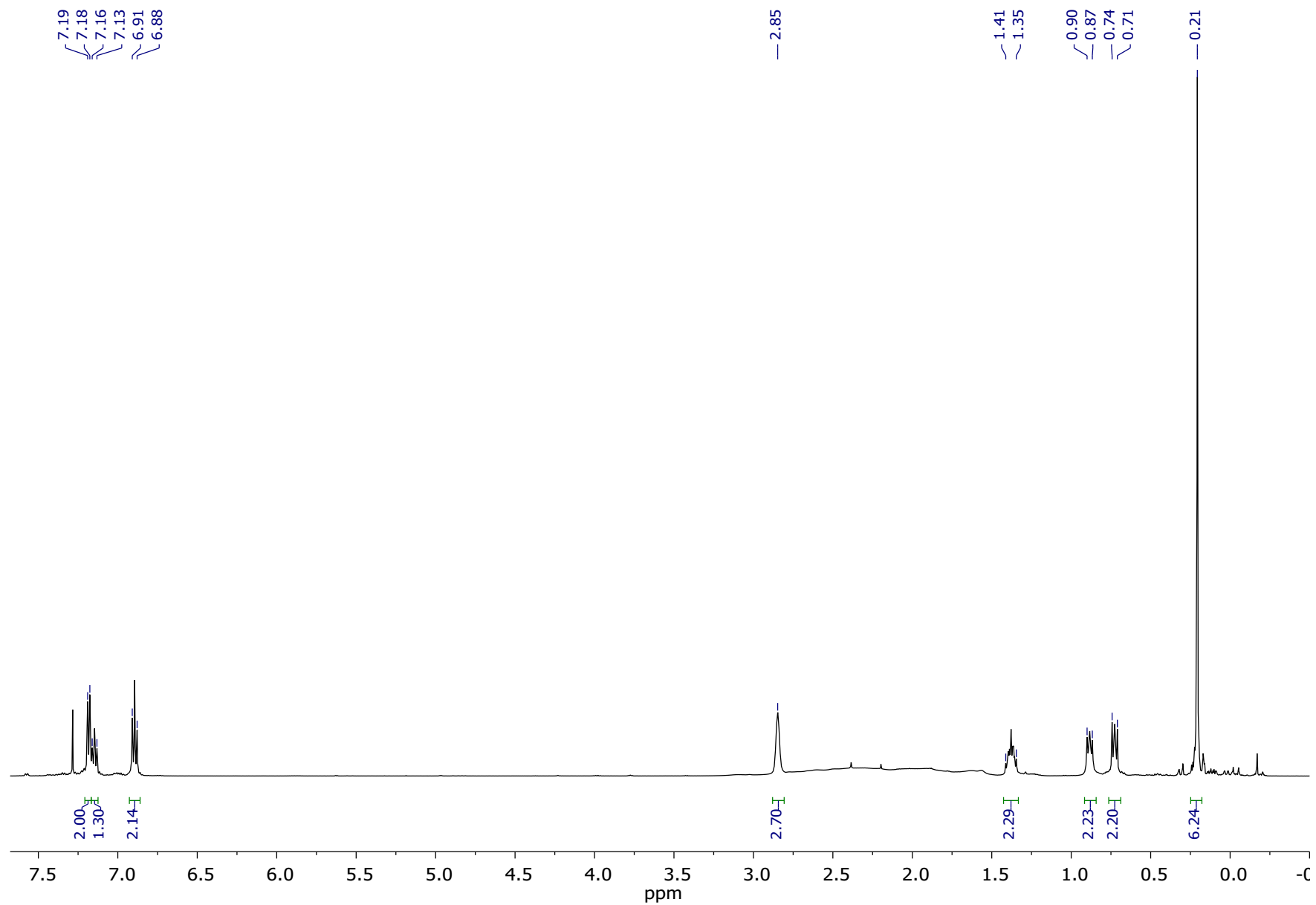


Fig S14. ¹H NMR (CDCl₃) spectrum of *cis*-hexa[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclohexasiloxane (cycle 6)

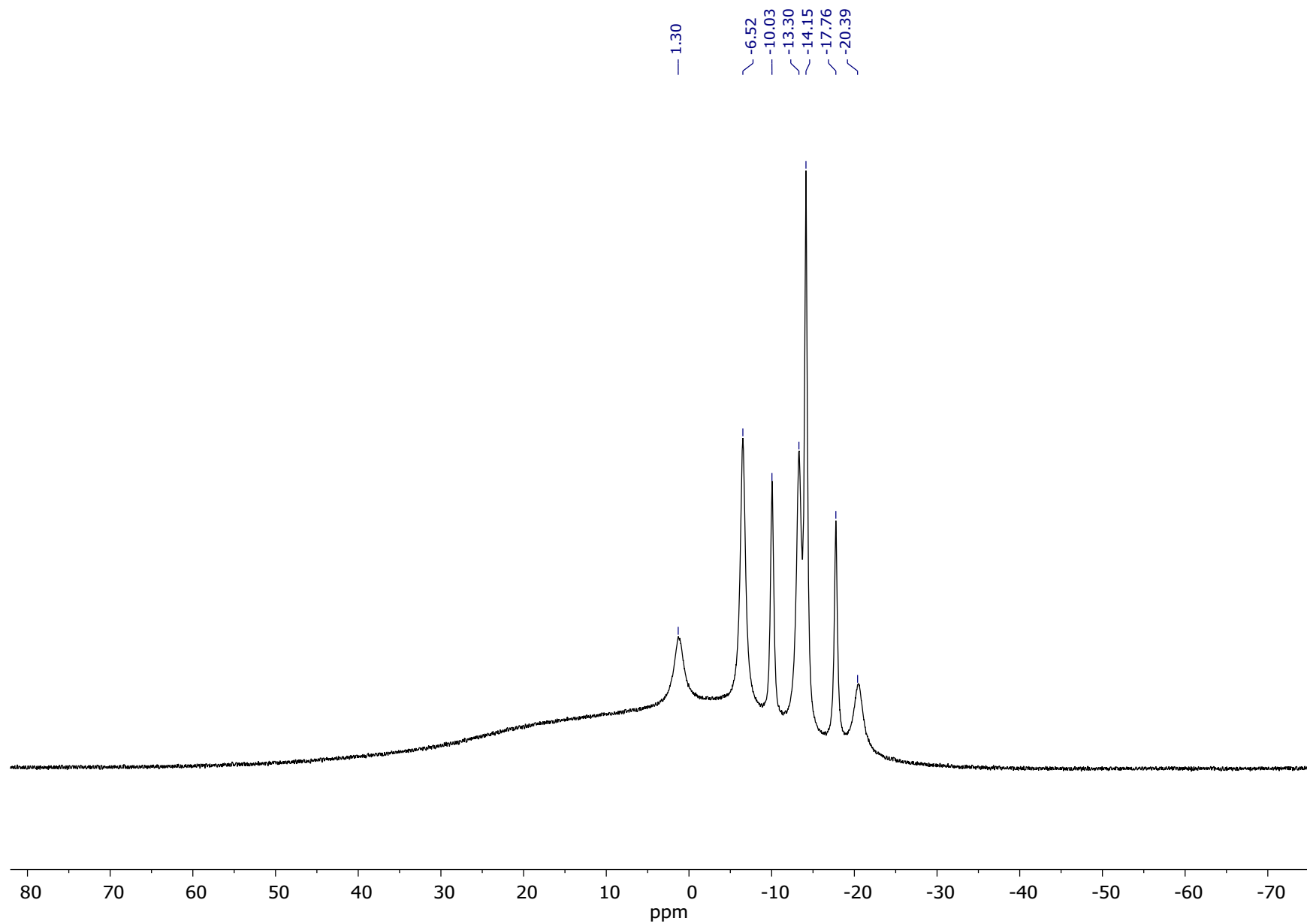


Fig S15. ^{11}B NMR (CDCl_3) spectrum of *cis*-hexa[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclohexasiloxane (cycle 6)

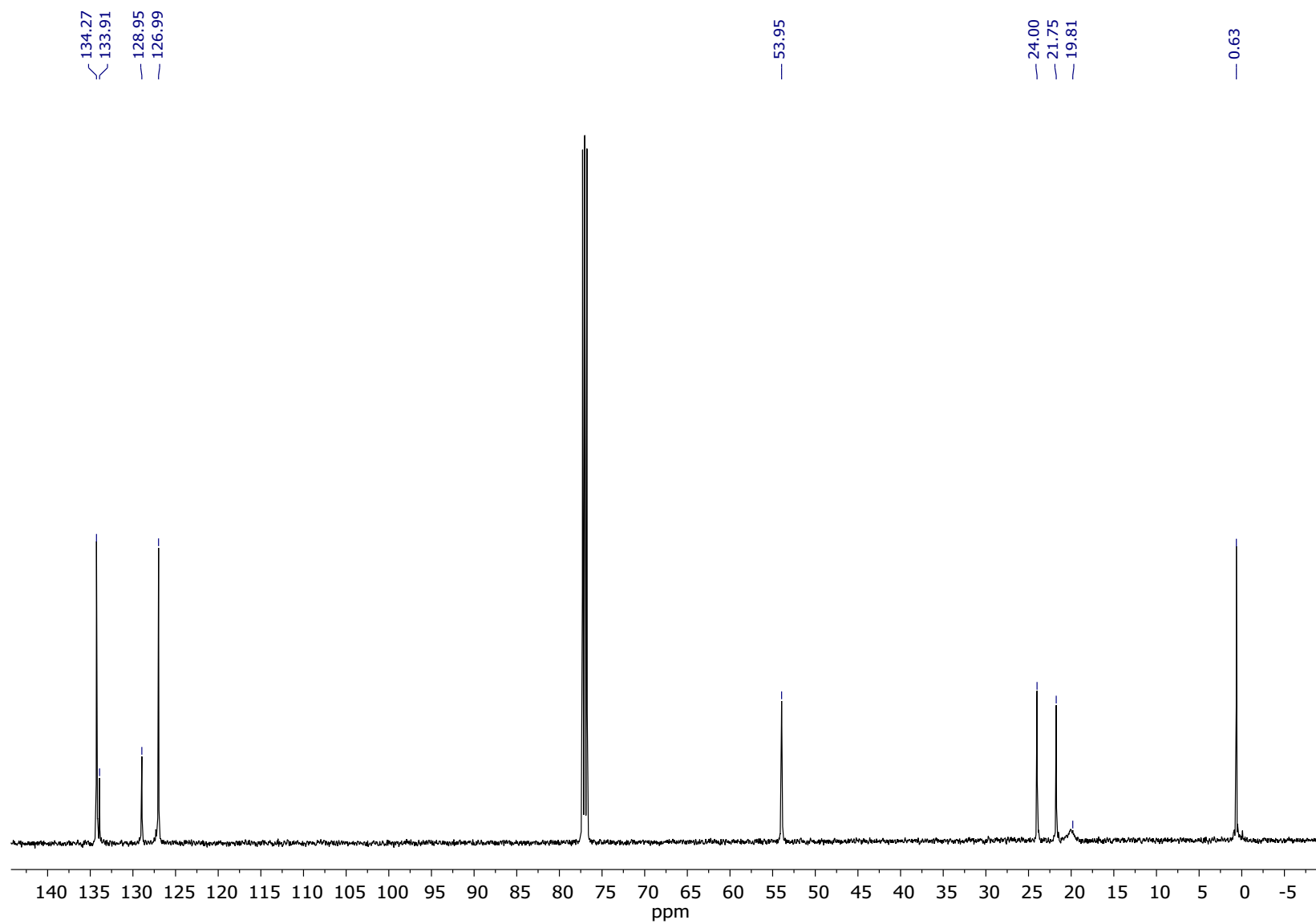


Fig S16. ^{13}C NMR (CDCl_3) spectrum of *cis*-hexa[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclohexasiloxane (cycle 6)

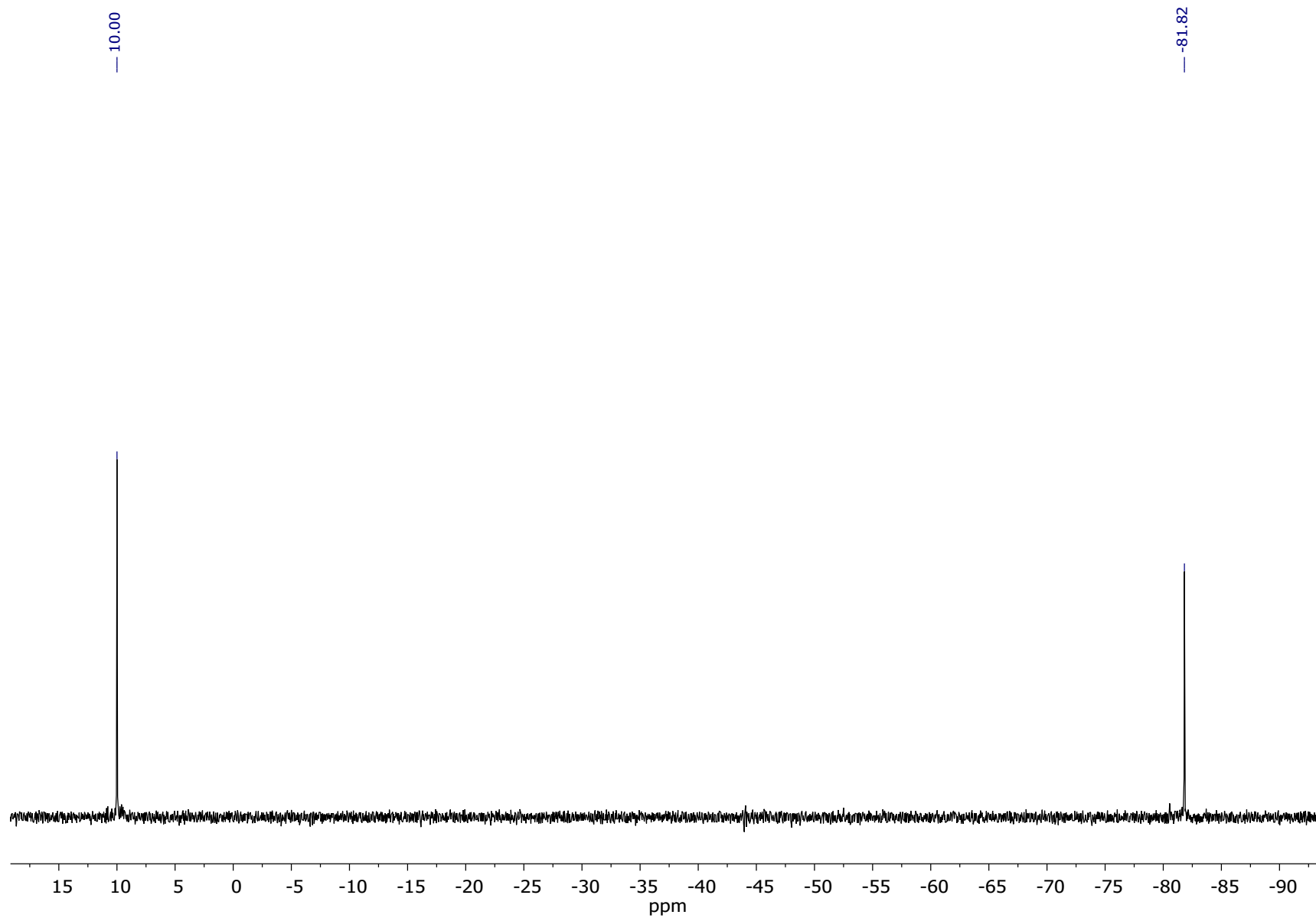


Fig S17. ^{29}Si NMR (CDCl_3) spectrum of *cis*-hexa[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclohexasiloxane (cycle 6)

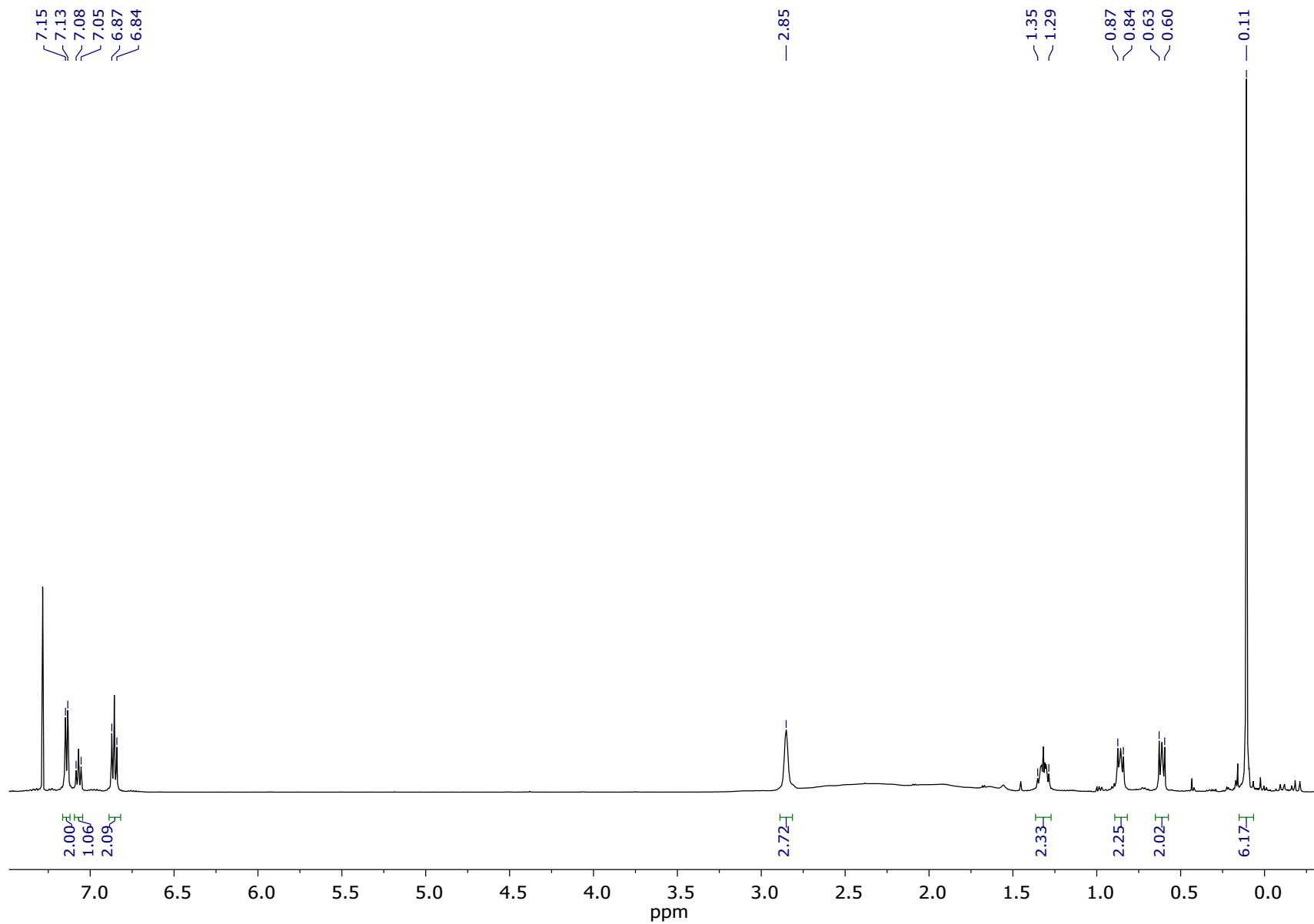


Fig S18. ^1H NMR (CDCl_3) spectrum of *cis*-octa[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclooctasiloxane (cycle 8)

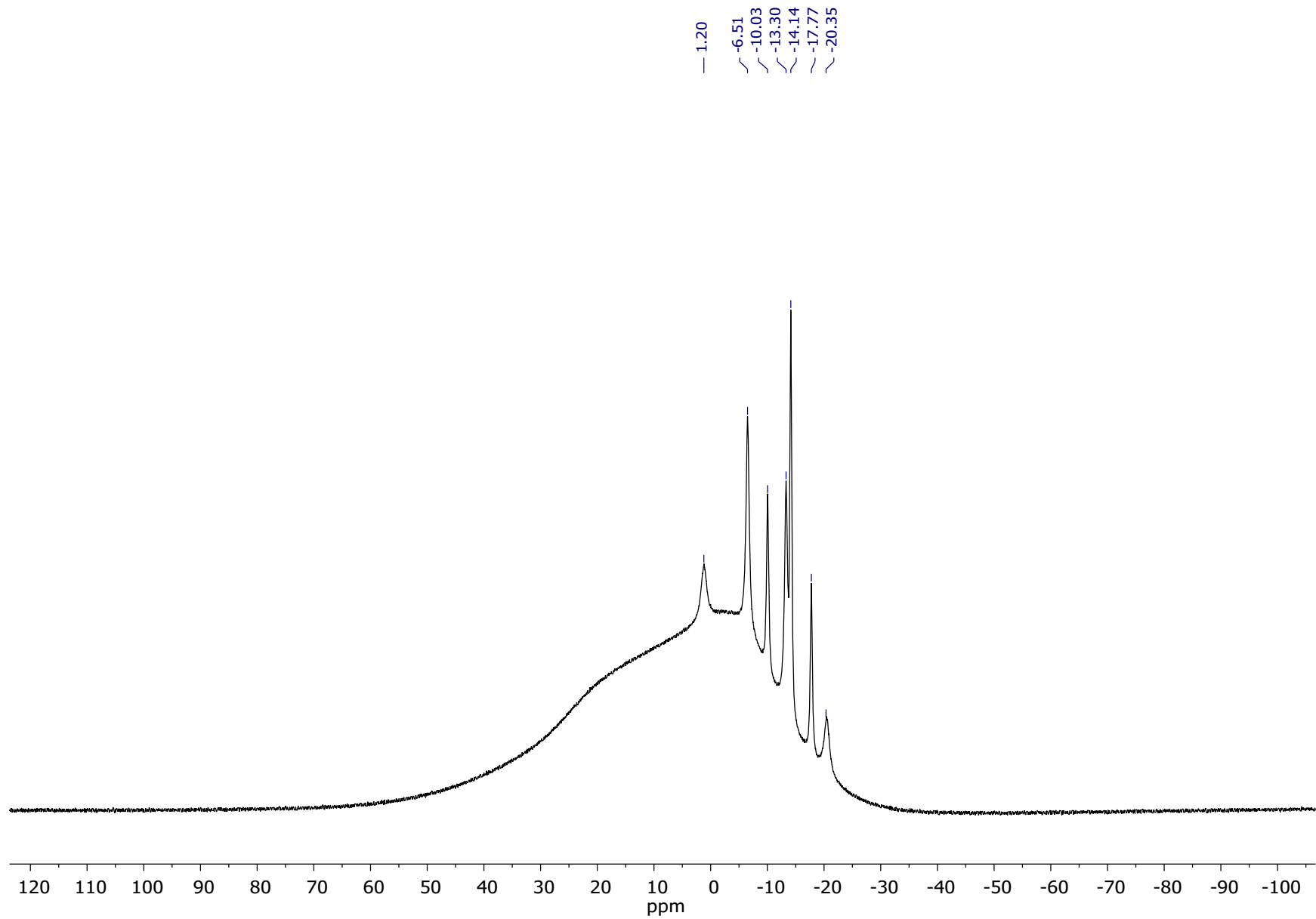


Fig S19. ^{11}B NMR (CDCl_3) spectrum of *cis*-octa[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclooctasiloxane (cycle 8)

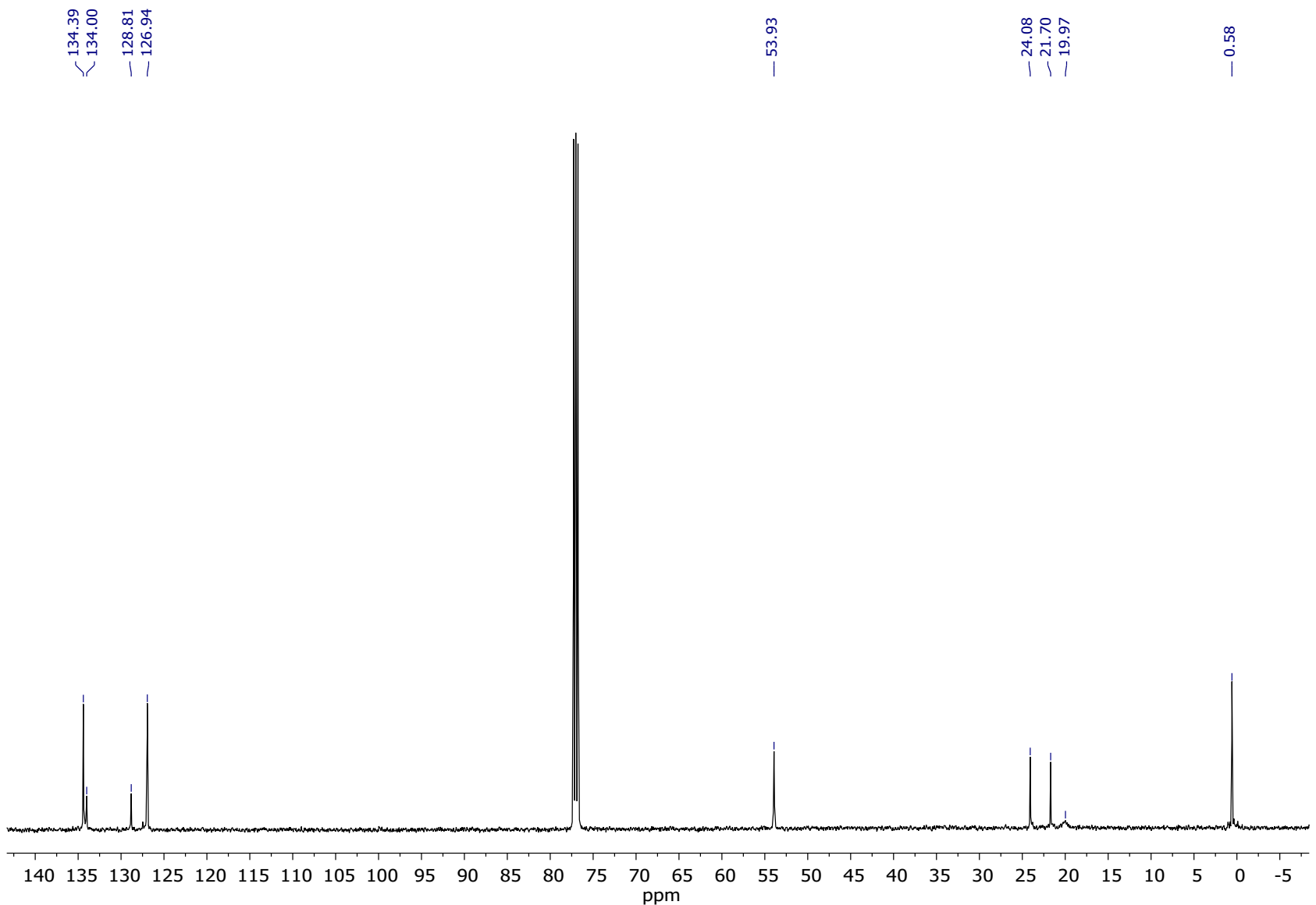


Fig S20. ^{13}C NMR (CDCl_3) spectrum of *cis*-octa[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclooctasiloxane (cycle 8)

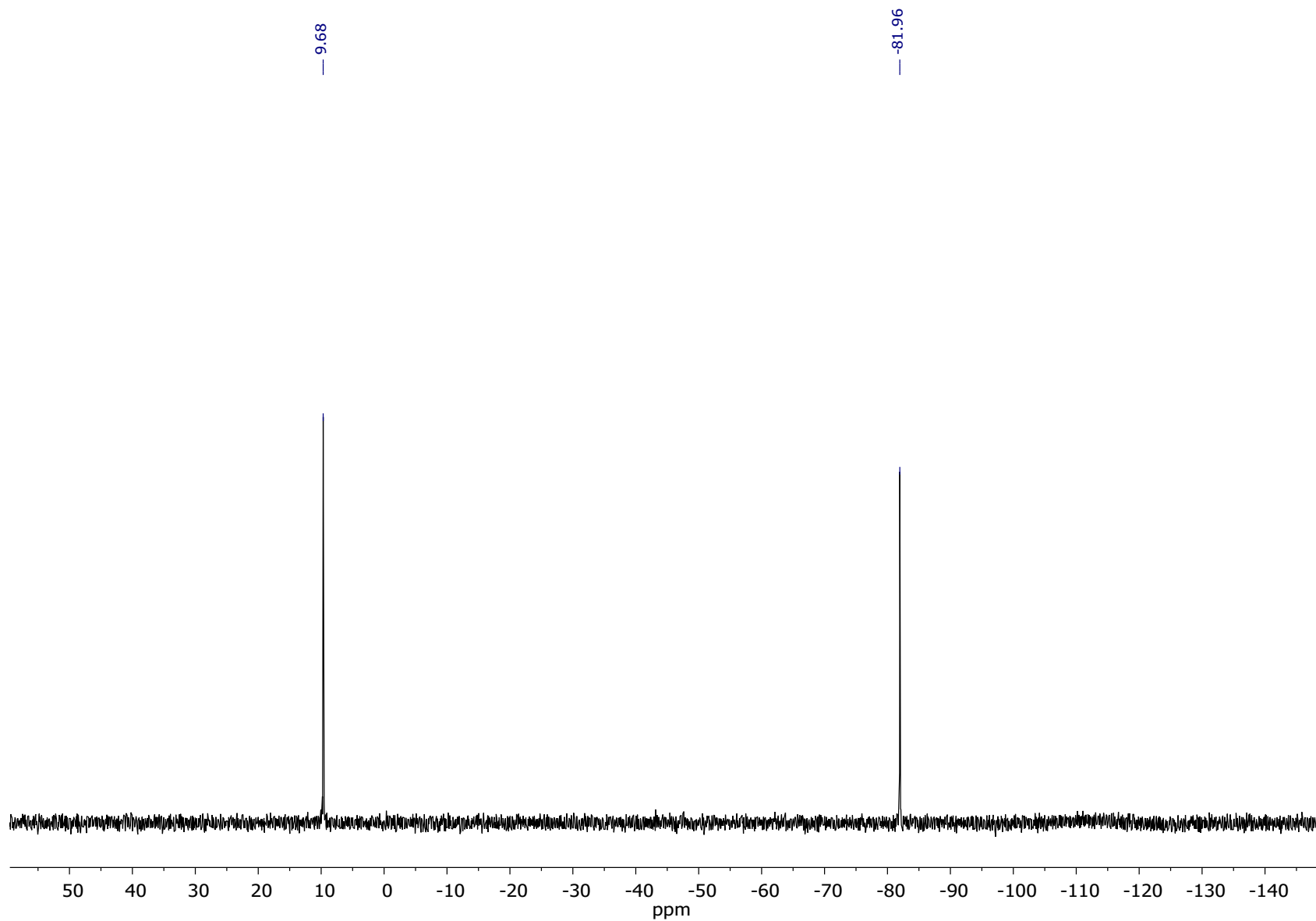


Fig S21. ^{29}Si NMR (CDCl_3) spectrum of *cis*-octa[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclooctasiloxane (cycle 8)

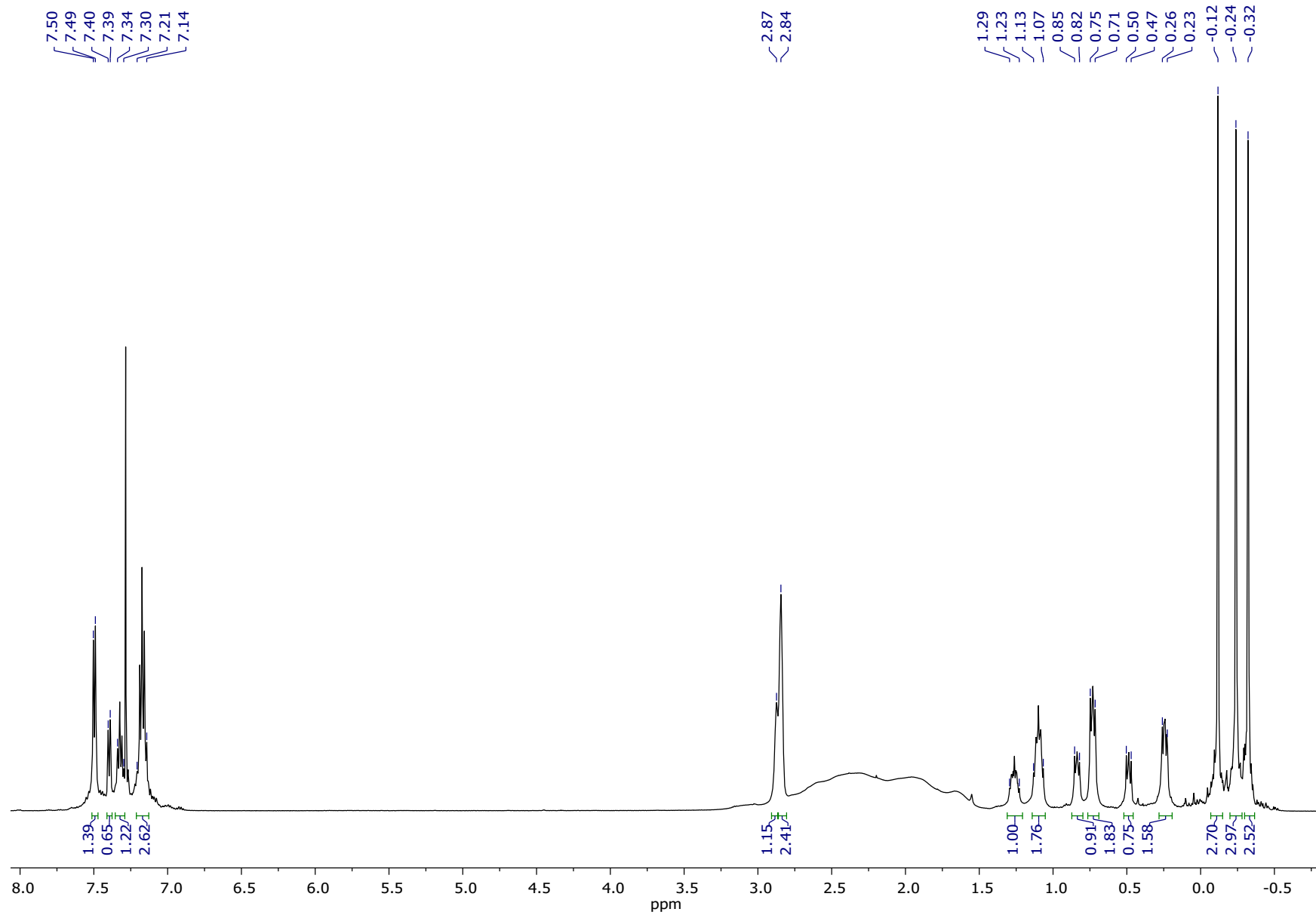


Fig S22. ^1H NMR (CDCl_3) spectrum of tris-*cis*-tris-*trans*-dodeca[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclododecasiloxane (cycle 12)

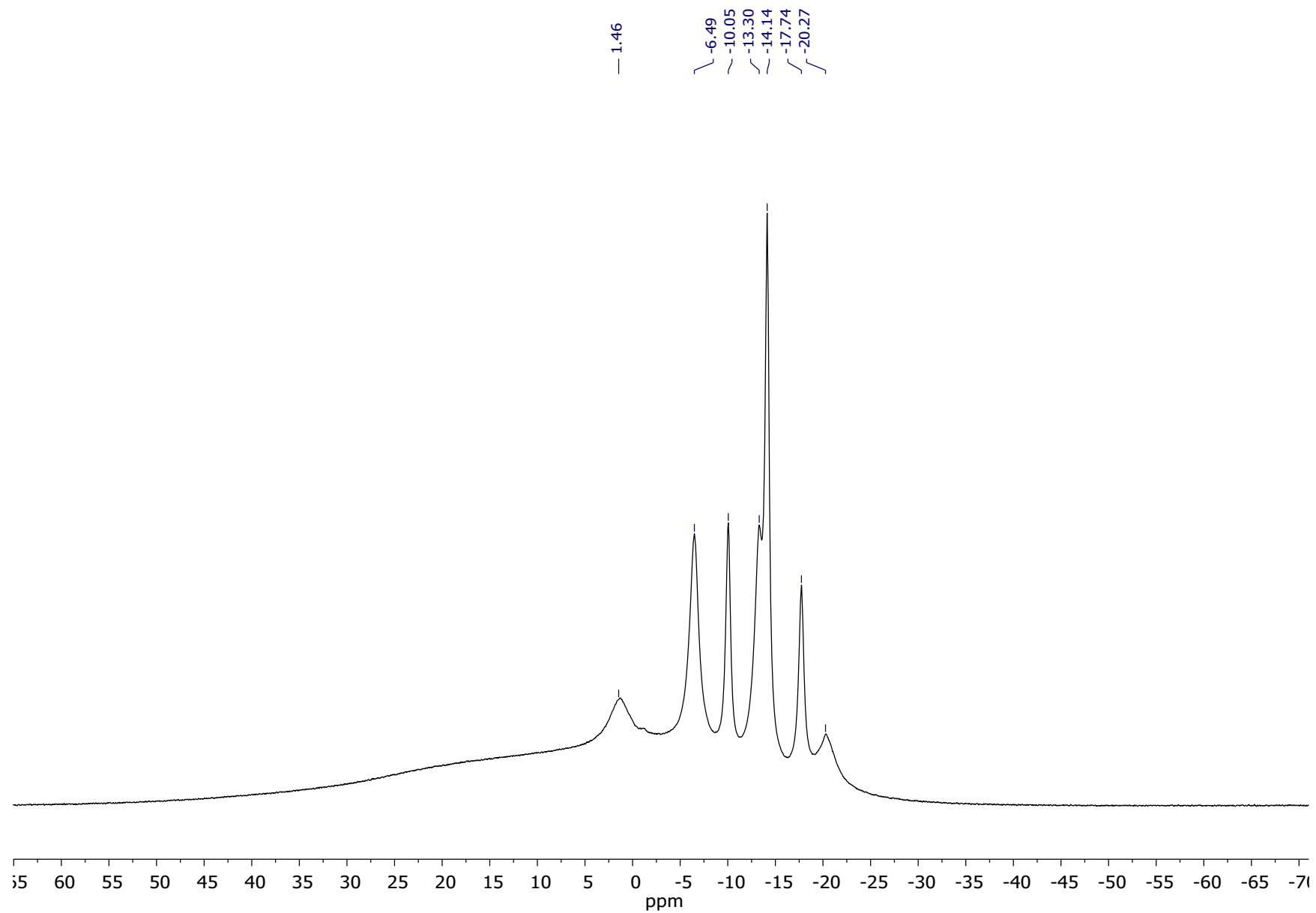


Fig S23. ^{11}B NMR (CDCl_3) spectrum of tris-*cis*-tris-*trans*-dodeca[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclododecasiloxane (cycle 12)

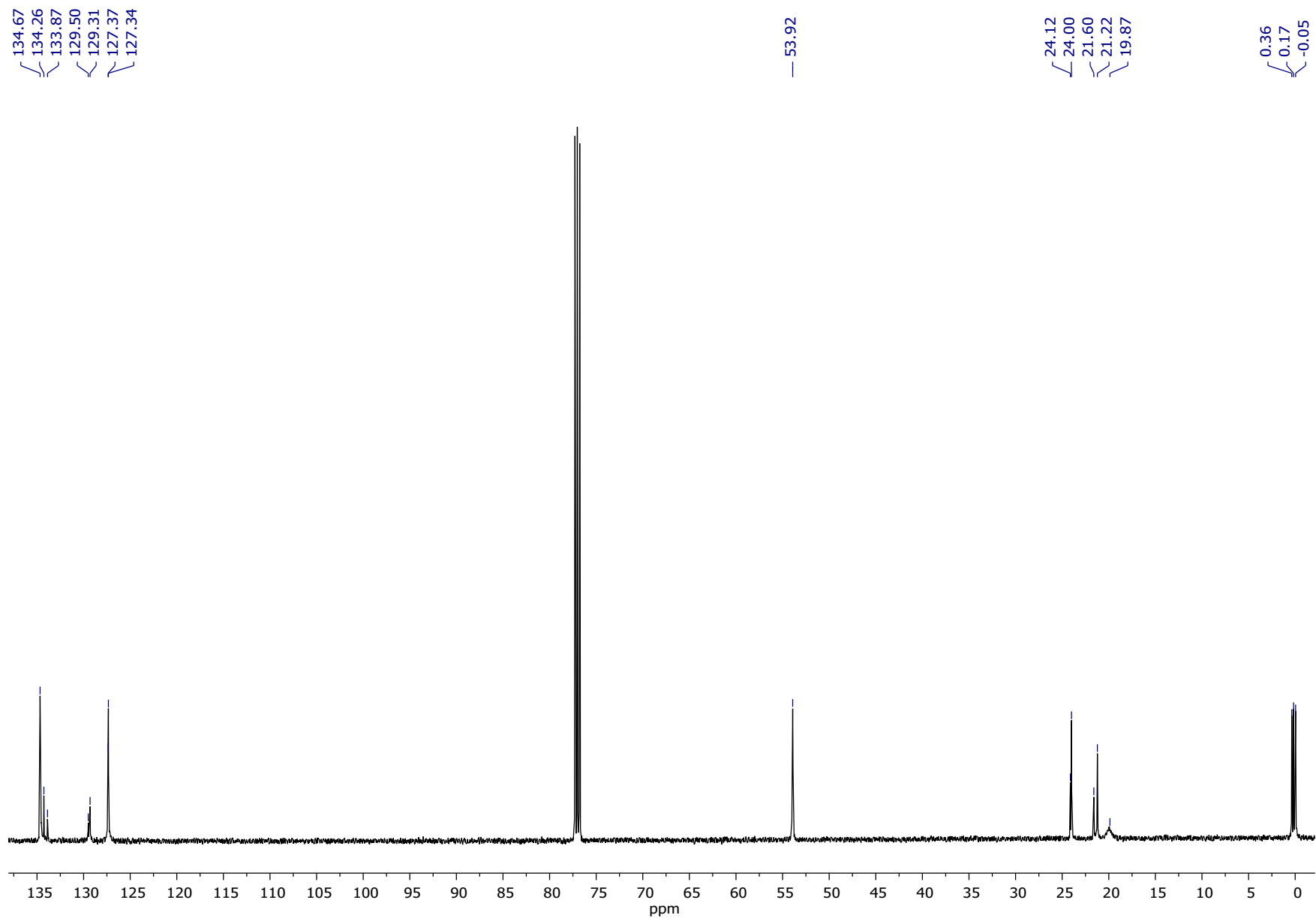


Fig S24. ^{13}C NMR (CDCl_3) spectrum of tris-*cis*-tris-*trans*-dodeca[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclododecasiloxane (cycle 12)

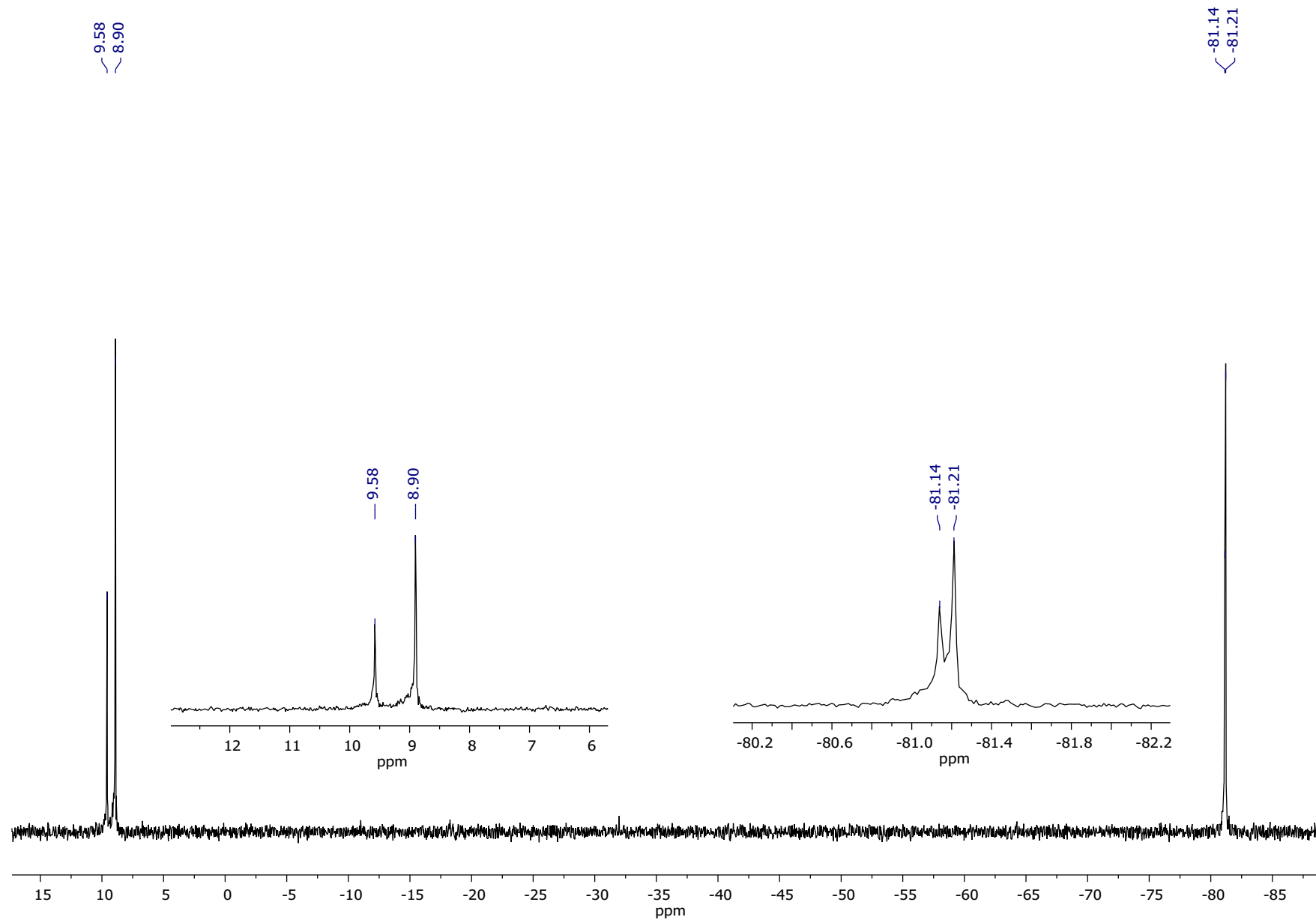


Fig S25. ^{29}Si NMR (CDCl_3) spectrum of tris-*cis*-tris-*trans*-dodeca[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclododecasiloxane (cycle 12)

IR spectra

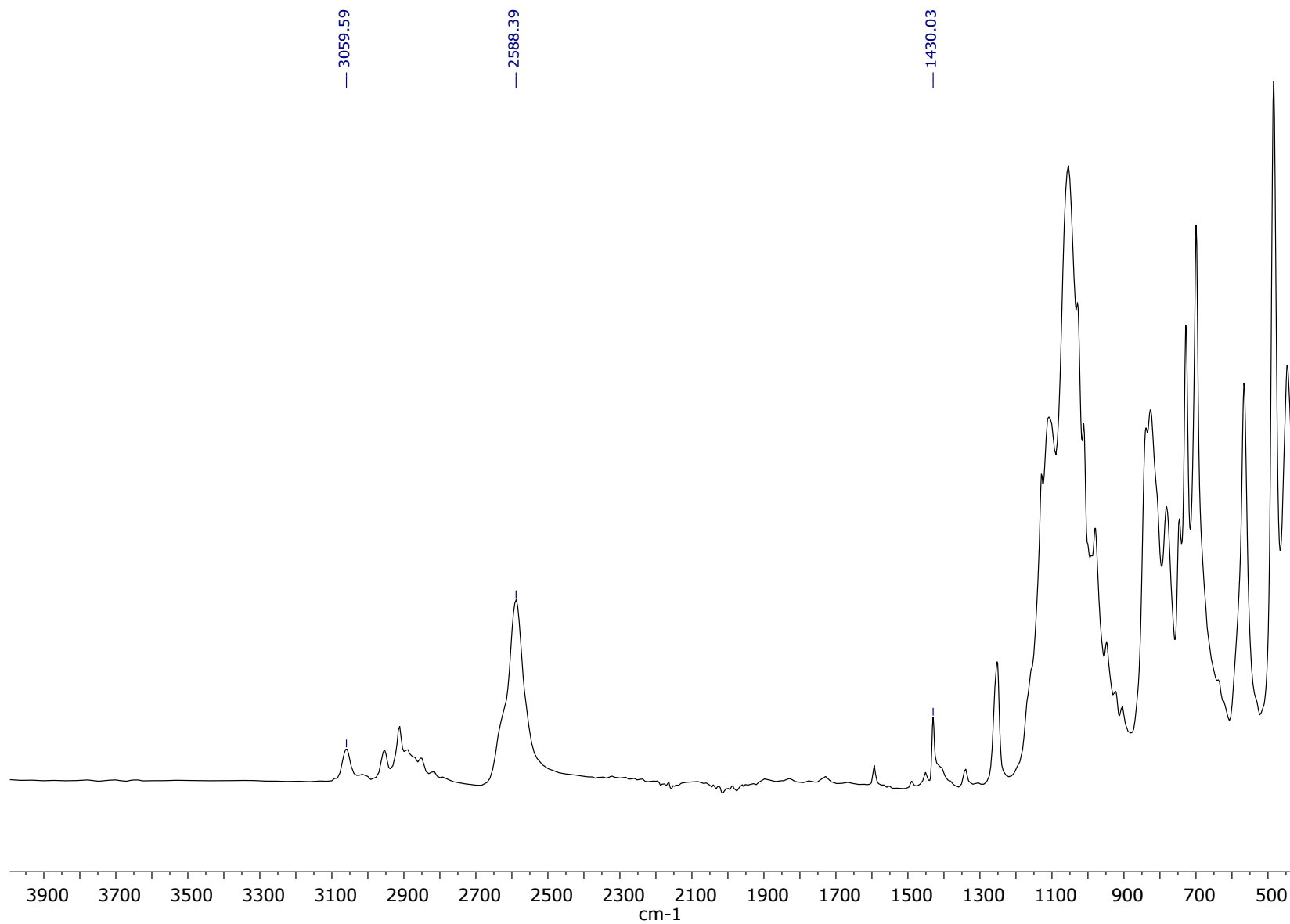


Fig S26. IR (cm⁻¹) spectrum of *cis*-tetra[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclotetrasiloxane (cycle 4)

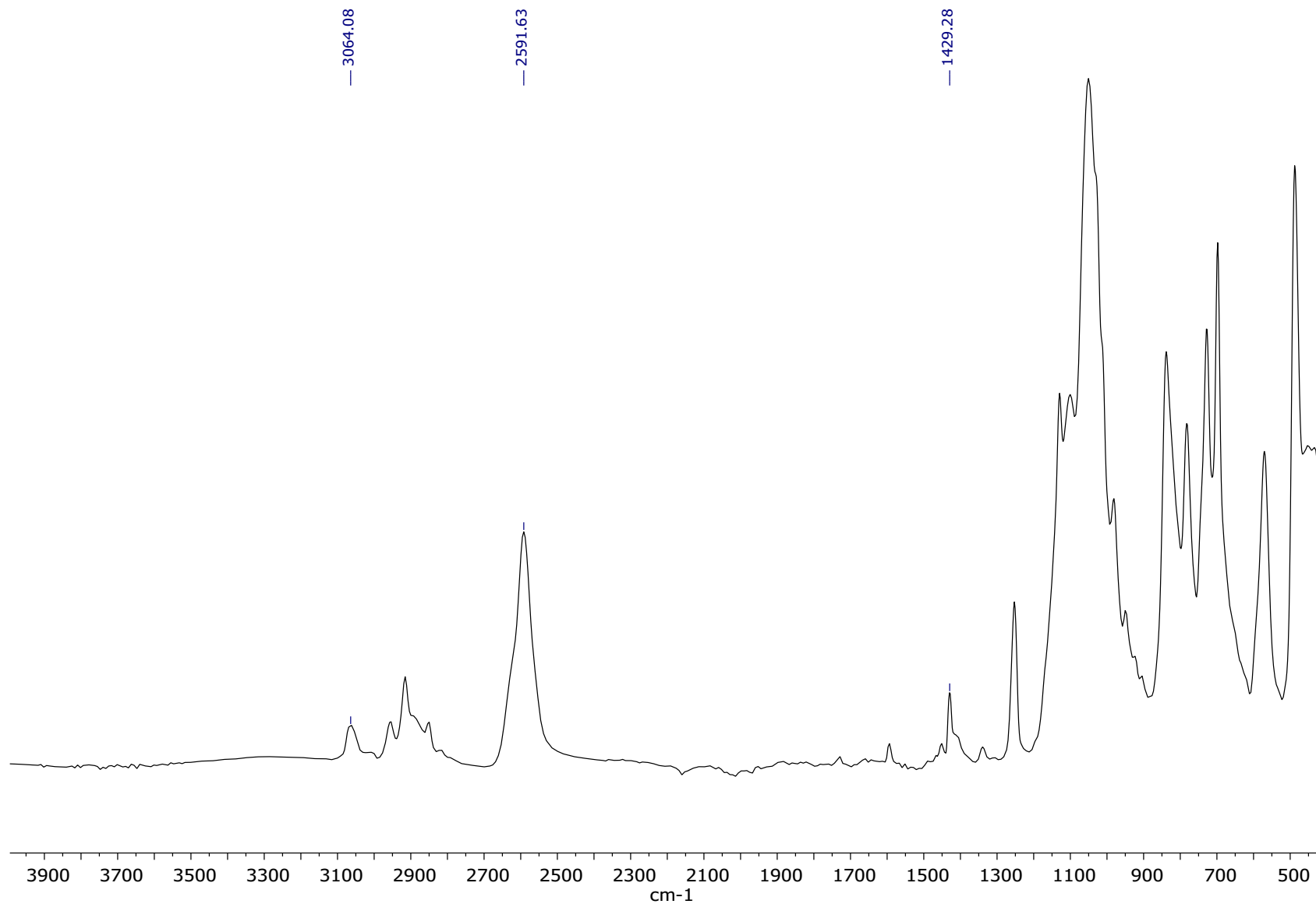


Fig S27. IR (cm⁻¹) spectrum of *cis*-penta[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclopentasiloxane (cycle 5)

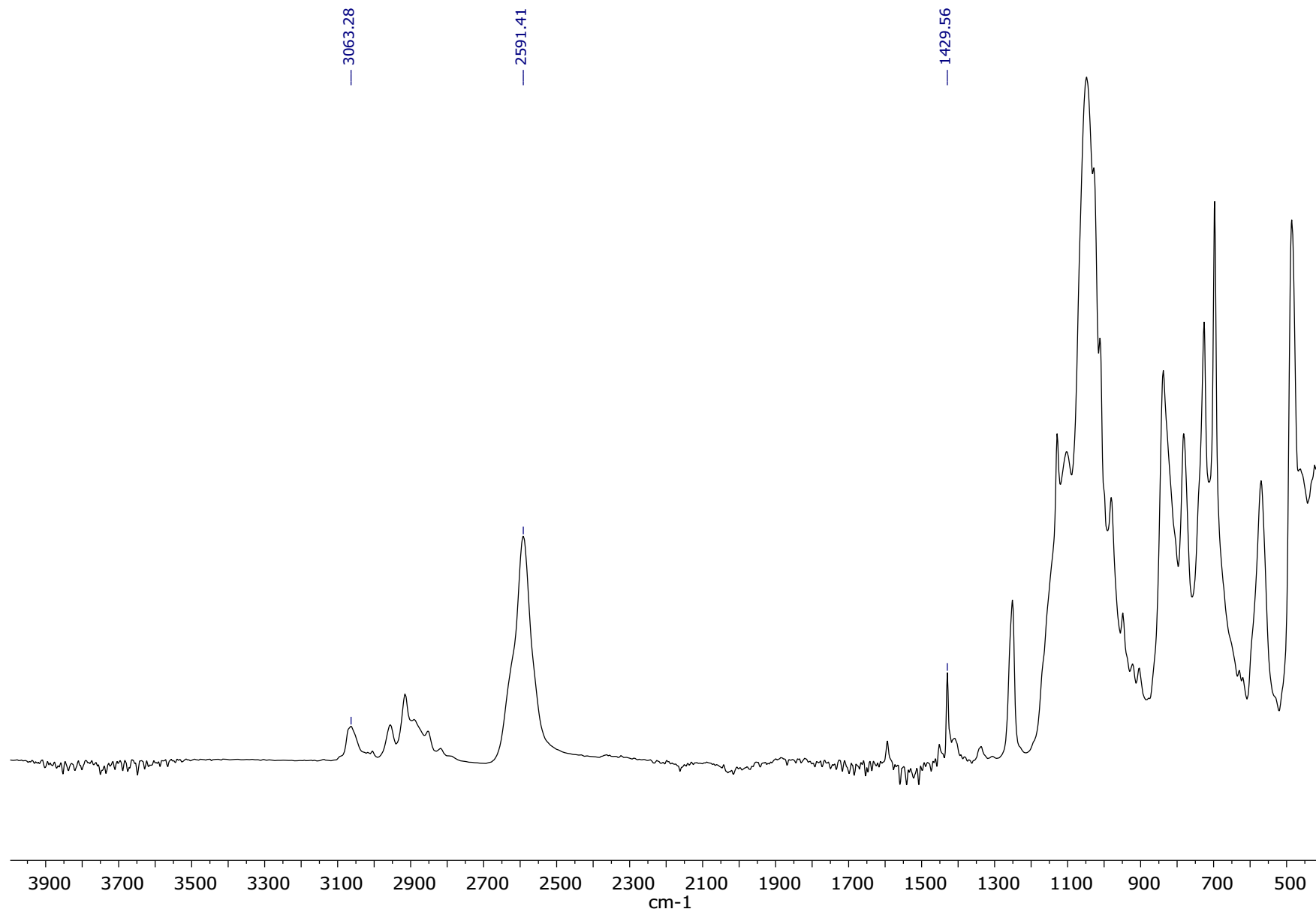


Fig S28. IR (cm⁻¹) spectrum of *cis*-hexa[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclohexasiloxane (cycle 6)

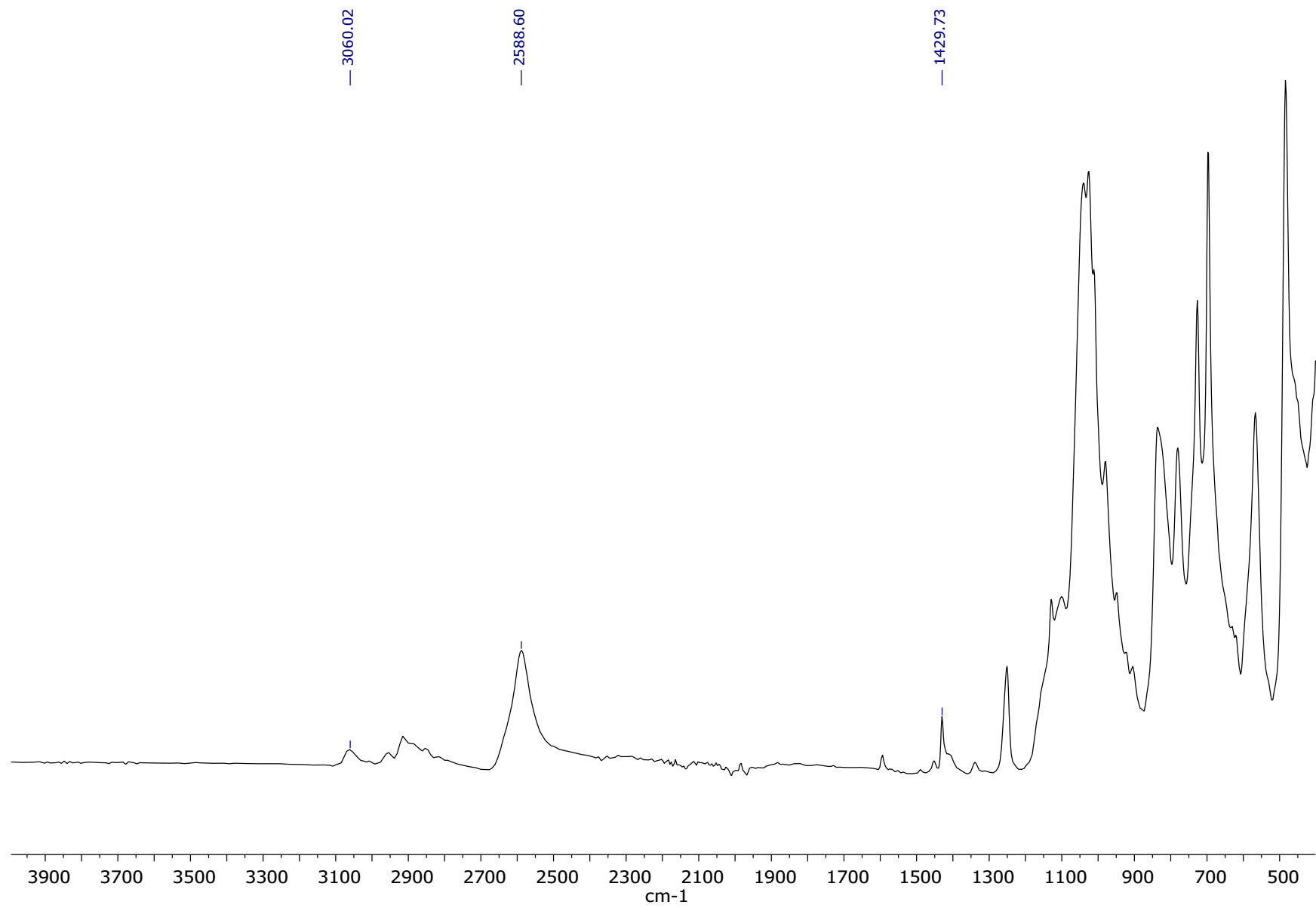


Fig S29. IR (cm⁻¹) spectrum of *cis*-octa[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclooctasiloxane (cycle 8)

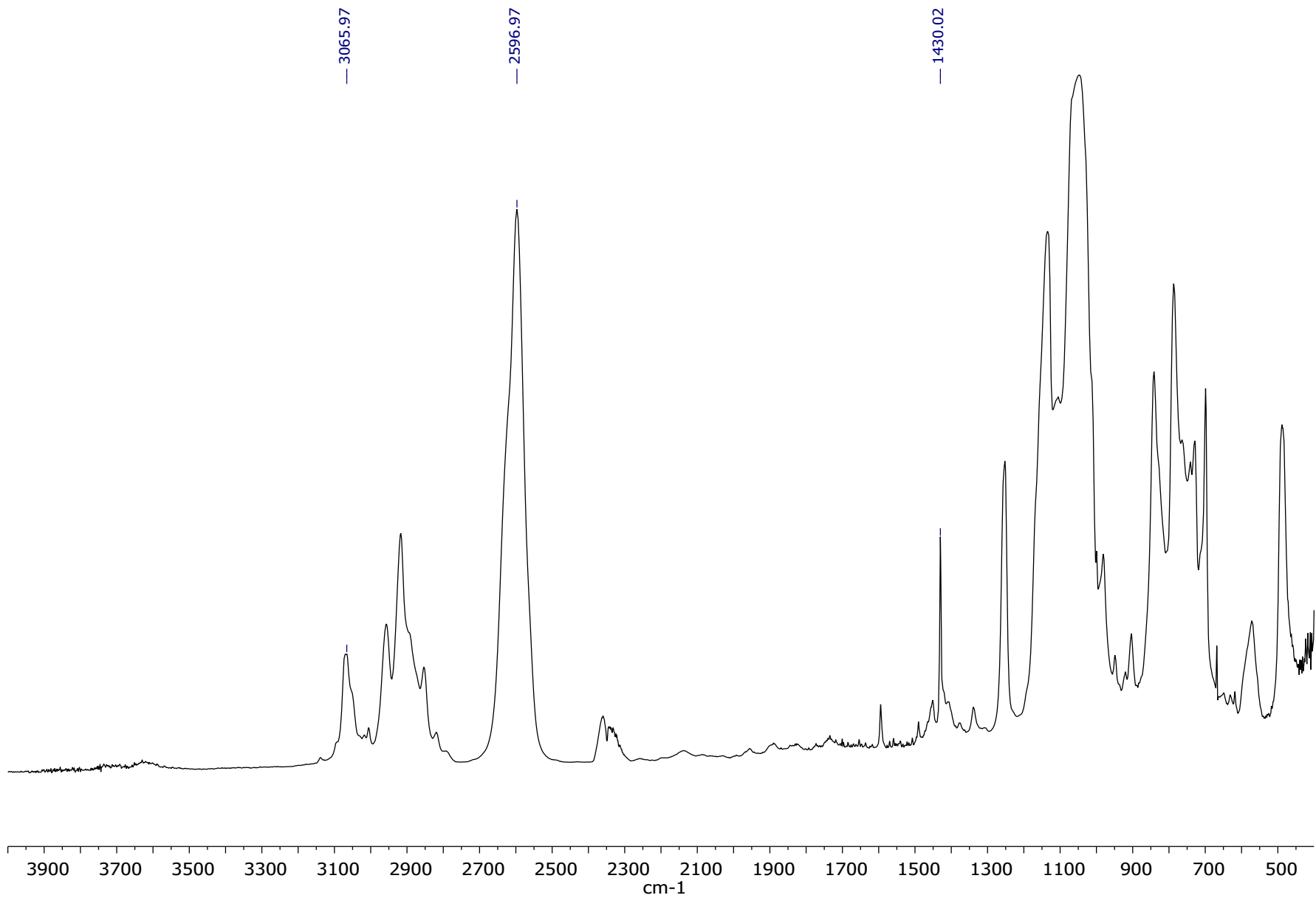


Fig S30. IR (cm⁻¹) spectrum of tris-*cis*-tris-*trans*-dodeca[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclododecasiloxane (cycle 12)

GPC data

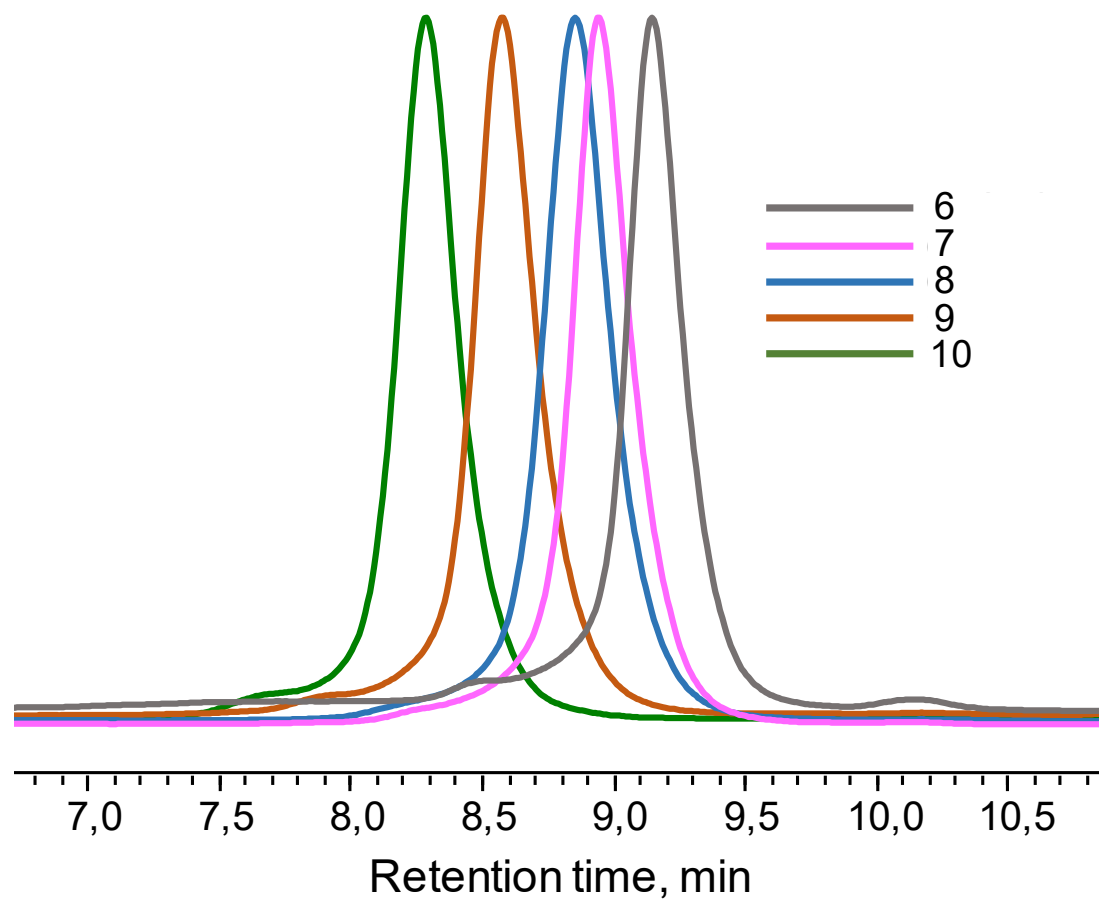


Fig S31. GPC curves of carboranophenylcyclsiloxanes

TGA data

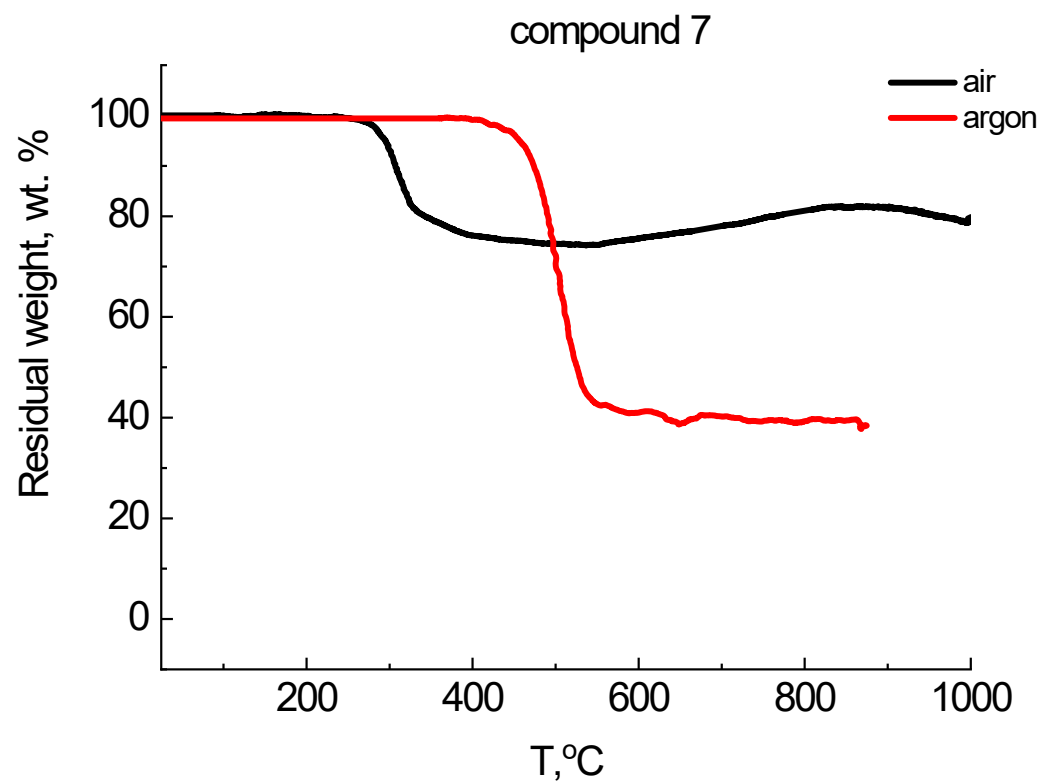


Fig S32. TGA curves of *cis*-penta[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclopentasiloxane in air (black curve) and in argon (red curve) at a heating rate of 10 °C/min

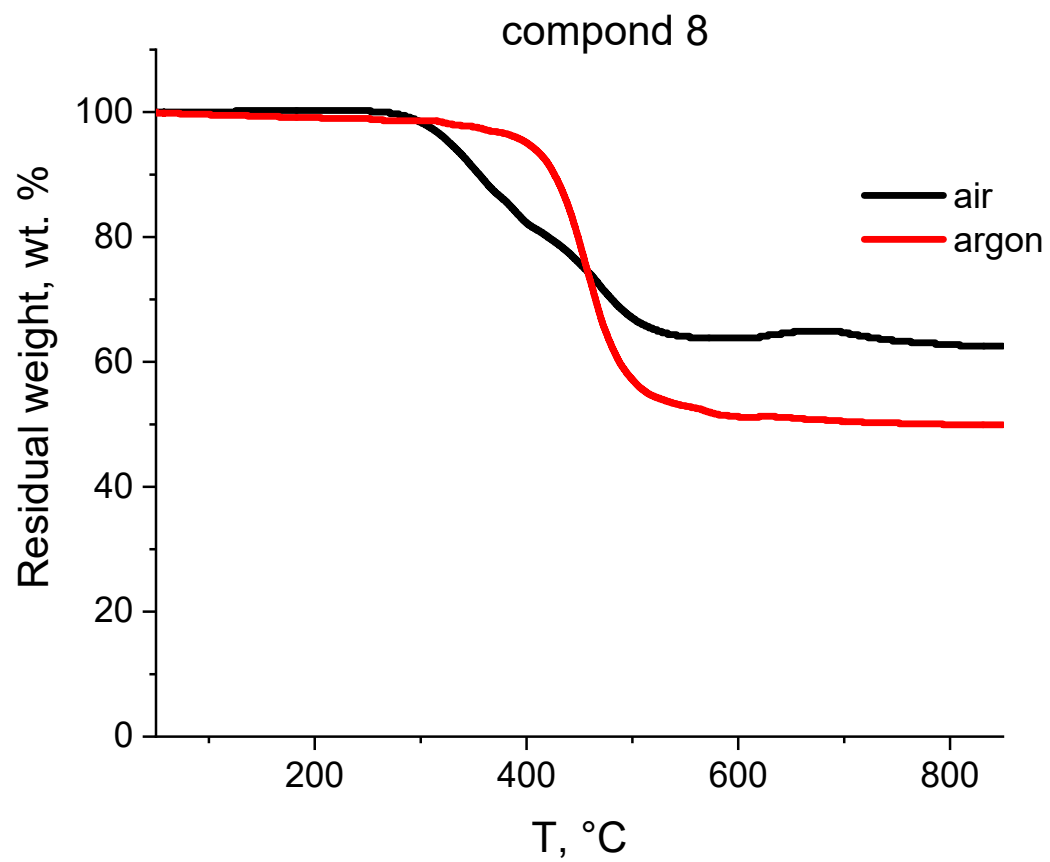


Fig S33. TGA curves of *cis*-hexa[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclohexasiloxane in air (black curve) and in argon (red curve) at a heating rate of 10 °C/min

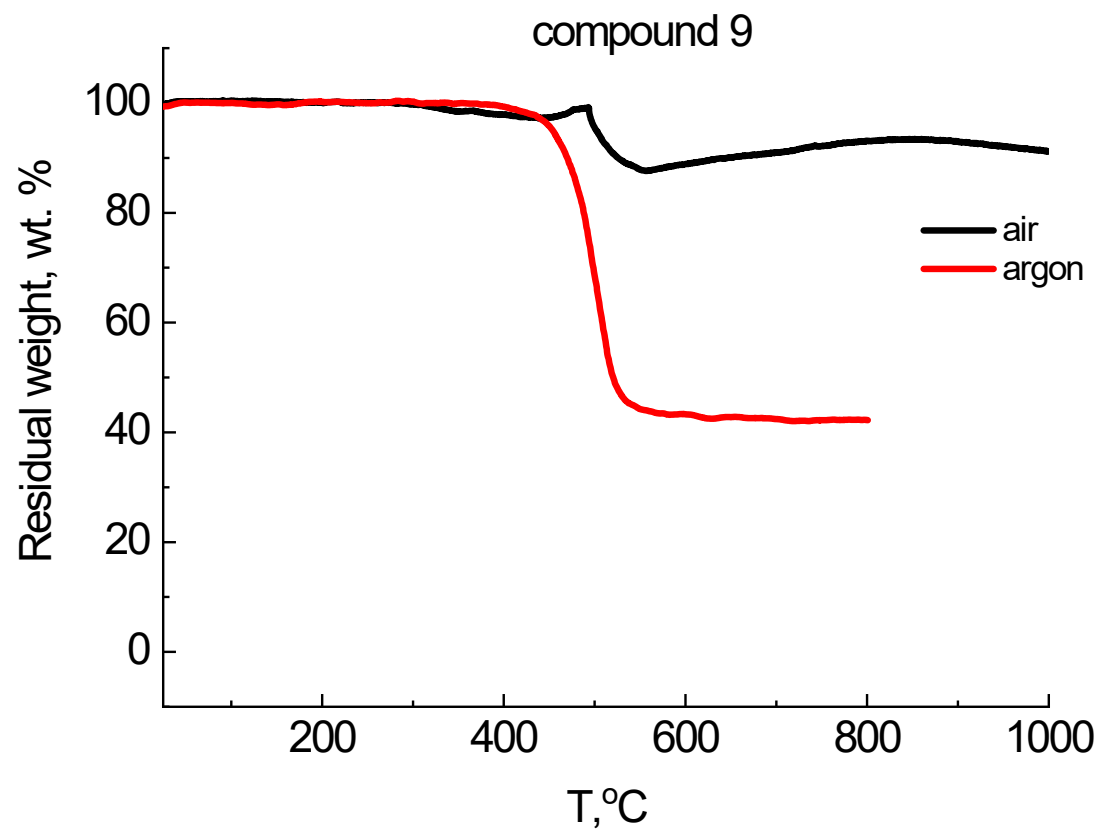


Fig S34. TGA curves of *cis*-octa[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclooctasiloxane in air (black curve) and in argon (red curve) at a heating rate of 10 °C/min

Mass spectra

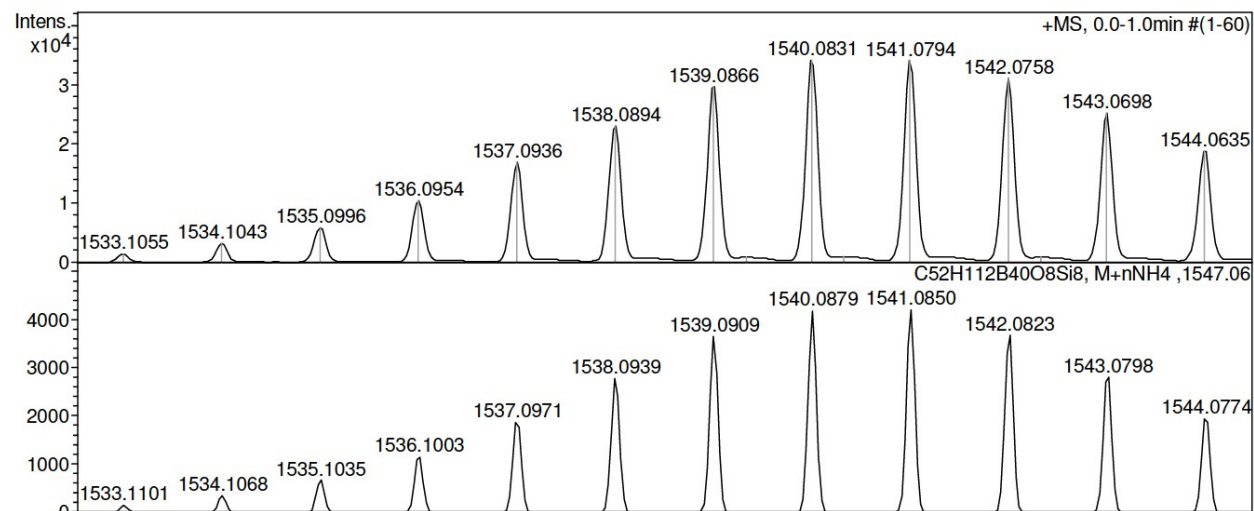


Fig S35. Mass spectrum of *cis*-tetra[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclotetrasiloxane (cycle 4)

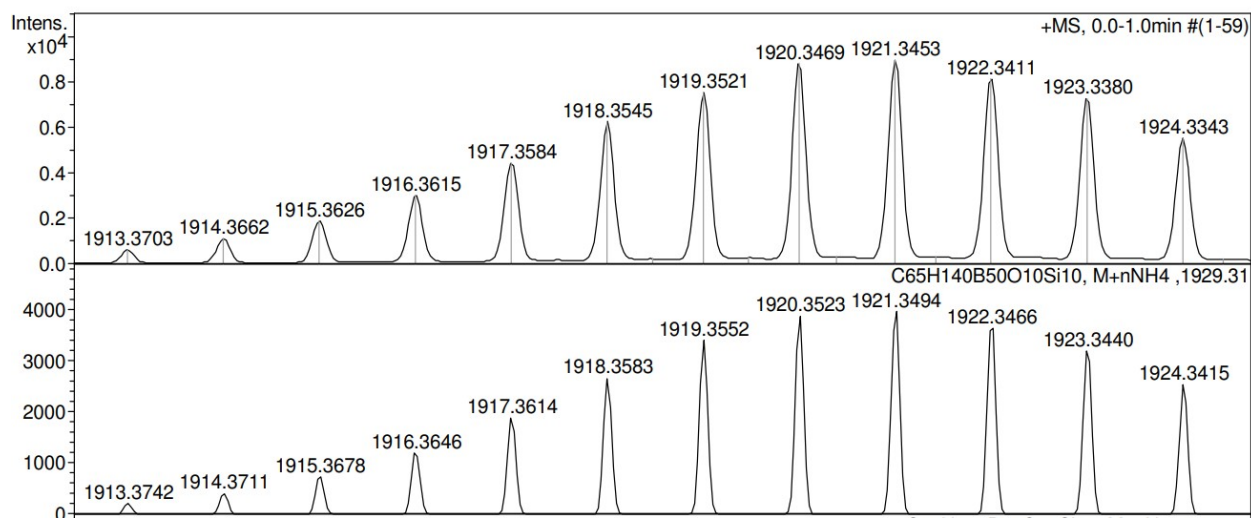


Fig S36. Mass spectrum of *cis*-penta[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclopentasiloxane (cycle 5)

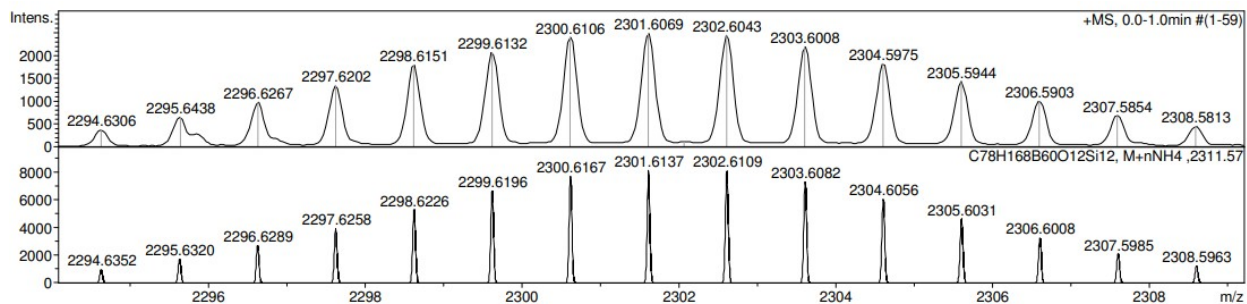


Fig S37. Mass spectrum of *cis*-hexa[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclohexasiloxane (cycle 6)

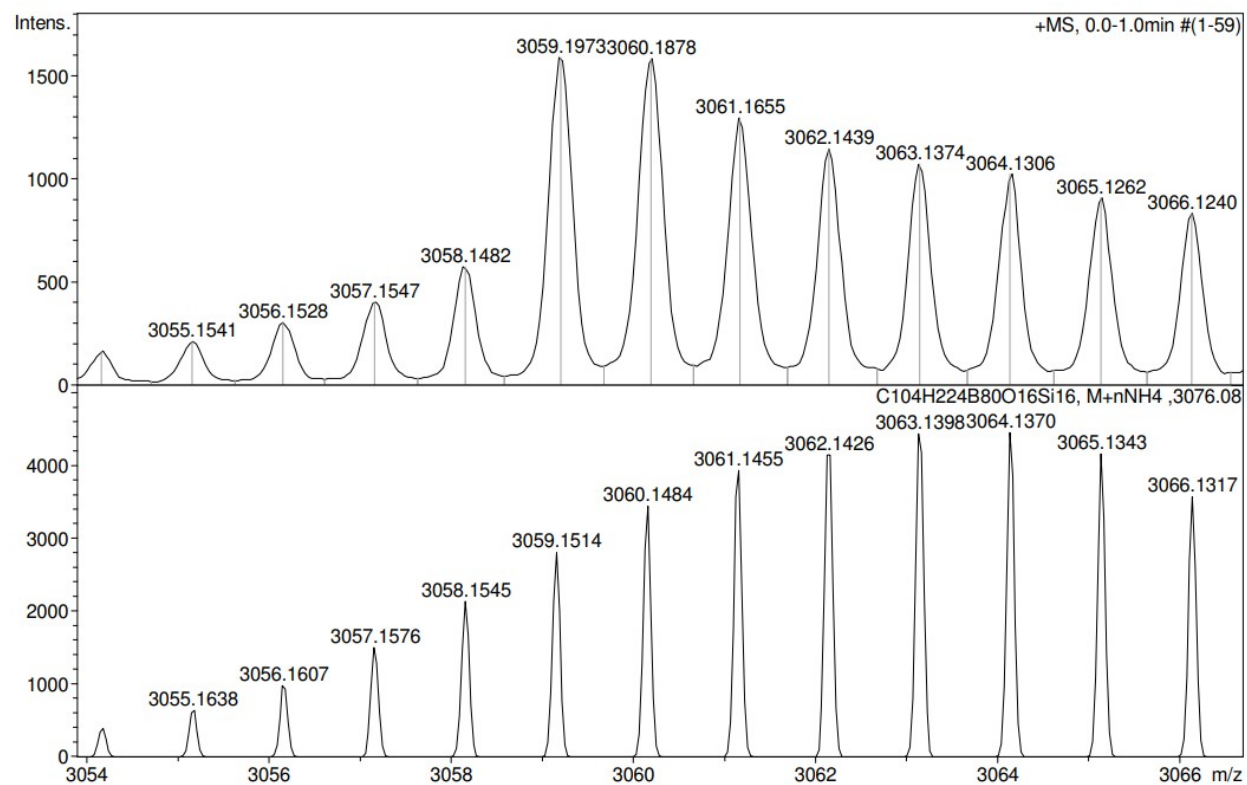


Fig S38. Mass spectrum of *cis*-octa[phenyl(1(3-(9-*m*-carboranyl)propyl)dimethylsiloxy)]cyclooctasiloxane (cycle 8)