

Supplementary Information

**Unlocking Regioselectivity: Steric Effects and
Conformational Constraints of Lewis Bases in
Alkylolithium-Initiated Butadiene
Polymerization**

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11 iPrDiPz, conformation 1.....	277
11 iPrDiPz, conformation 2.....	278
11 iPrDiPz, transition state 1-2	280

Temperature Effects on 1,2-Selectivity in Lewis Base/RLi Systems

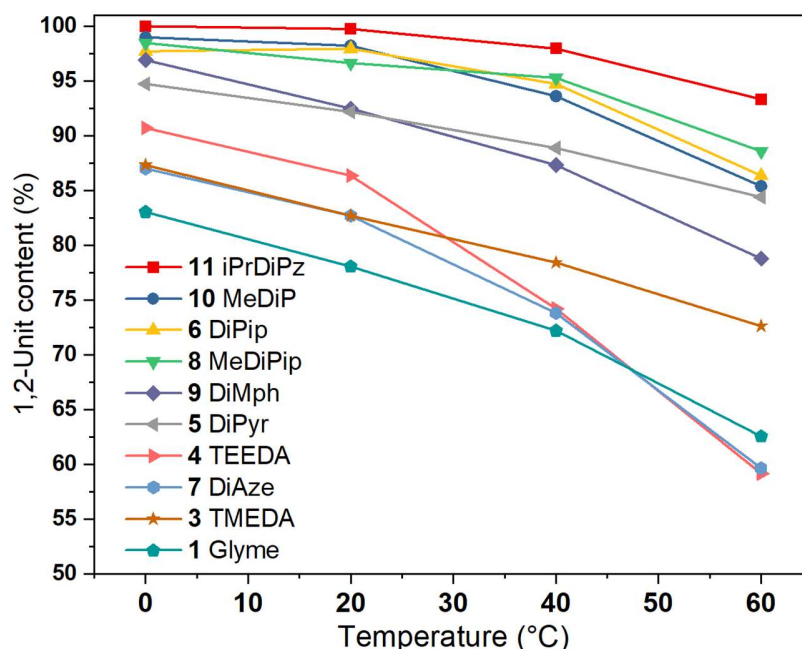


Figure S1. Effect of temperature on the 1,2-unit content in polybutadiene in the presence of different Lewis bases

To explore the effectiveness and universality of the conformational constraint effect in Lewis base/*t*-BuLi systems over a broader range of conditions, we evaluated the 1,2-selectivity in the polymerization of butadiene initiated by various systems composed of Lewis bases and tert-butyllithium at 0°C, 20°C, 40°C, and 60°C. The solvent **2** THF was excluded from this experiment due to the extremely short half-life of alkylolithium in **2** THF at high temperatures, leading to rapid active species deactivation. Except for temperature variations, the polymerization conditions matched those in Table 1 of the main text.

Figure S1 reveals that Lewis bases **11**, **10**, **8**, and **6**, which exhibit strong conformational constraint effects, consistently achieve optimal 1,2-selectivity across both low and high temperatures, with the disparity becoming more significant at elevated temperatures. At 60°C, non-conformationally constrained Lewis bases **7** DiAze, **4** TEEDA, **3** TMEDA, and **1** glyme demonstrate poor 1,2-selectivity, with the lowest being merely 60%. Conversely, Lewis bases **11**, **10**, **8**, and **6**, which possess strong conformational constraint effects, maintain regioselectivity above 85% at 60°C. Particularly noteworthy is **11** iPrDiPz, which, despite having the highest conformational change energy, achieves an impressive 93% 1,2-selectivity at 60°C (98% at 40°C), surpassing all previously reported anionic polymerization systems. Furthermore, Lewis bases **5** and **9**, which exhibit moderate conformational constraint effects, show 1,2-selectivity that lies between the strongly and weakly constrained Lewis bases. The strength of the conformational constraint effect is quantitatively reflected by the conformational change energy

barrier, as detailed in Figure 6 of the main text.

These results indicate that initiator systems comprising Lewis bases with conformational constraint effects exhibit superior 1,2-selectivity across both high and low temperatures.

^{13}C NMR spectra of deuterium-labeled chain-end polybutadiene

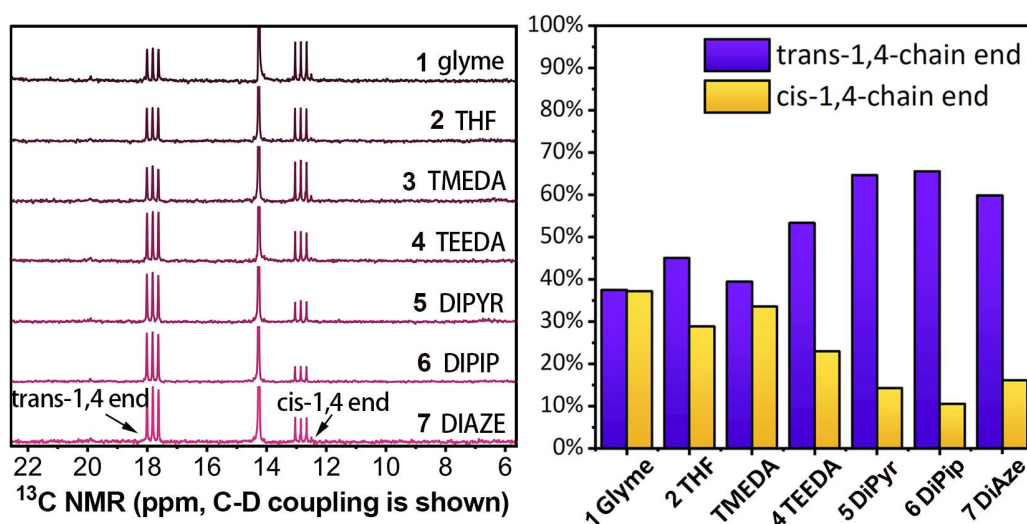


Figure S2. ^{13}C NMR spectra of deuterium-labeled chain-end polybutadiene.

To further characterize the polybutadiene quenched with deuterated methanol as shown in Figure 2 of the main text, we recorded the ^{13}C NMR spectra to observe carbon-deuterium coupling. As depicted in Figure S2, although the ratio of 1,2- to 1,4-end groups in the polybutadiene obtained after quenching with different Lewis bases is relatively consistent, there are significant differences in the cis/trans ratio of the 1,4-end groups. In general, bulkier Lewis bases tend to result in a higher proportion of trans-1,4-end groups. This observation is consistent with the conclusions drawn from the in situ ^{13}C NMR analysis (Figure 8).

Comparison of ^{13}C NMR and ^2H NMR Analyses in Charge

Distribution Characterization

In this study, we employed both ^{13}C NMR and ^2H NMR spectroscopy to investigate the charge distribution at the chain-end allylic carbanion during the anionic polymerization of 1,3-butadiene in the presence of various Lewis bases. While both methods provided valuable insights and led to consistent conclusions regarding the influence of electronic effects on regioselectivity, quantitative differences were observed between the two techniques. This section discusses these differences in detail.

The ^{13}C NMR measurements were conducted on the "live" polymerization systems without quenching, allowing direct observation of the charge distribution among the α -, β -, and γ -carbons of the chain-end allylic carbanion. The negative charge is delocalized over these three positions, and the chemical shifts of the α - and γ -carbons are sensitive indicators of electron density.

However, the β -carbon signal overlaps with the signals from the backbone double bonds of polybutadiene, which appear around 130 ppm. This overlap makes it challenging to isolate and quantify the β -carbon's contribution to the overall charge distribution. Consequently, the ^{13}C NMR analysis provides the relative ratio of electron density between the α - and γ -carbons, without accounting for the β -carbon.

The ^{13}C NMR results showed that, in the presence of various Lewis bases, the negative charge distribution between the γ - and α -carbons was approximately 4:6. This indicates that about 40% of the negative charge is localized at the γ -carbon, while 60% resides at the α -carbon.

For the ^2H NMR experiments, the polymerization reactions were quenched with methanol- d_4 (MeOD), resulting in deuterium-labeled polybutadiene. This approach indirectly probes the charge distribution by analyzing where deuterium atoms are incorporated into the polymer chain-end after quenching.

During the quenching process, the chain-end carbanion abstracts a deuteron (D^+) from MeOD. The β -carbon, being a secondary carbon already bonded to two other carbons, cannot form an additional bond with deuterium. Therefore, deuterium incorporation occurs primarily at the α - and γ -carbons. Any negative charge initially associated with the β -carbon is effectively redistributed to these positions during quenching. The ^2H NMR data revealed that, even after the addition of various Lewis bases, deuterium incorporation at the γ -position was approximately 25%, while about 75% was at the α -position. This suggests a preferential localization of the negative charge at the α -carbon during the quenching process.

This raises a further question: why is the β -carbon's charge preferentially transferred to the α -carbon rather than equally to both α - and γ -carbons after quenching? We hypothesize that this is due to the enhanced stability of the primary carbanion (1°C) at the α -position compared to the secondary carbanion (2°C) at the γ -position. Additionally, the steric environment at the α -carbon is less hindered, which promotes the "transfer" of the β -carbon's charge to the α -carbon. It's worth noting that "transfer" here may not be the most precise term; rather, it is the delocalization of negative charge over the β -carbon that facilitates electrophilic attack by D^+ at the α -carbon.

In summary, while both ^{13}C NMR and ^2H NMR analyses support the conclusion that electronic effects alone do not fully account for the enhanced 1,2-insertion observed, they provide different quantitative insights due to the nature of their measurement techniques. The ^{13}C NMR offers a direct observation of the live chain-end's electron distribution, whereas ^2H NMR reflects the charge distribution after quenching, influenced by factors such as carbanion stability and steric hindrance. Recognizing these differences is crucial for accurately interpreting the data and understanding the mechanisms underlying regioselectivity in anionic polymerization.

Comparison of DFT computational study and polymerization experiments on cis/trans-1,4 selectivity

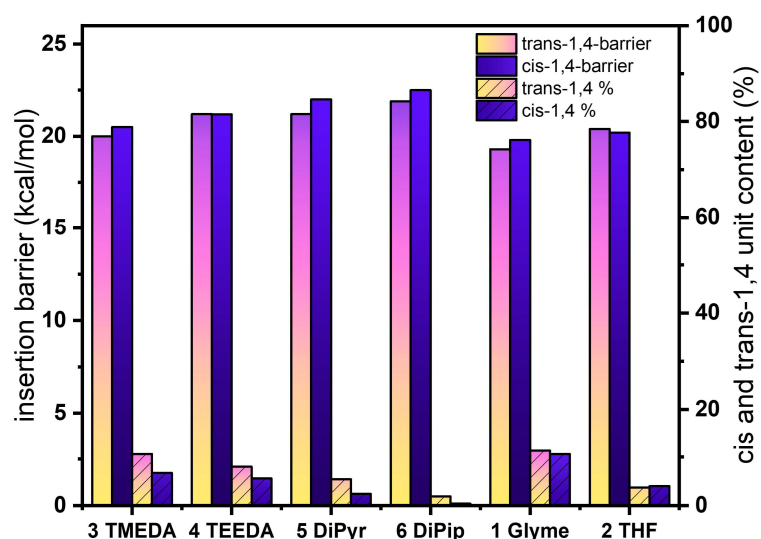


Figure S3. Correlation between DFT-calculated trans/cis-1,4-insertion barriers and trans/cis-1,4-unit content in polymerization products

Table S1. Relationship between DFT-computed trans/cis-1,4 insertion energy barriers and polymer microstructure ^[a]

Entry	Lewis base	Insertion barrier		Microstructure (%)			
		trans-1,4	cis-1,4	1,2	trans-1,4	cis-1,4	trans/cis
1	1 Glyme	19.3	19.8	78.1	11.3	10.6	1.1
2	2 THF ^[c]	20.4	20.2	91.3	3.7	4.0	0.9
3	3 TMEDA	20	20.5	82.7	10.6	6.7	1.6
4	4 TEEDA	21.2	21.1	86.4	8.0	5.6	1.4
5	5 DiPyr	21.2	22.0	92.2	5.4	2.4	2.3
6	6 DiPip	21.9	22.5	97.7	1.9	0.4	4.8

[a] Polymerization conditions: in n-hexane at 20 °C for 10 h. The microstructure of polymers was determined by ¹³C-NMR.

In the main text, we extensively discuss the relationship between the DFT-calculated 1,2-insertion energy barriers and the 1,2-unit content in the polymers obtained from polymerization experiments (as illustrated in Figure 5), which shows a pretty good correlation.

Similarly, the trans/cis-1,4 unit ratio in the polymers correlates strongly with the DFT-calculated trans/cis-1,4 insertion energy barriers. The energy barriers for cis-1,4 and trans-1,4 insertions, as calculated by DFT, are very close (with a much smaller difference compared to the 1,2- and 1,4-insertion barriers), not exceeding 1 kcal/mol. This small difference is anticipated, given that the content

difference between cis-1,4 and trans-1,4 units in the polymer is also less than 3%. The DFT-calculated data qualitatively align with the polymerization experiment results. However, considering the current precision limitations in computational chemistry, such a small energy barrier difference (less than 1 kcal/mol) may carry a relatively significant error margin. Nevertheless, the DFT results align remarkably well with the experimental outcomes. For instance, **6** DiPip and **5** DiPry, which exhibit conformational constraint effects, show lower trans-1,4 insertion energy barriers, resulting in a higher trans-1,4-unit content compared to cis-1,4 units in the respective polymers. In contrast, **1** glyme and **2** THF, with lower steric hindrance, exhibit minimal differences in cis/trans-1,4 insertion energy barriers. The actual polymer products show nearly equivalent cis/trans-1,4-unit content.

Furthermore, as depicted in Figure 7 of the main text, the disparity in cis/trans-1,4 insertion energy barriers is attributed to the differing steric requirements of the anti/syn-allyl isomers. Specifically, the anti-allyl isomer requires more space than the syn-isomer. Hence, when the ligand is a bulky or conformationally constrained Lewis base (such as **6** DiPip), the active species tend to favor the syn conformation, leading to the formation of trans-1,4 units.

Investigation of Polymer End Groups and Repeating Units by MALDI-TOF-MS

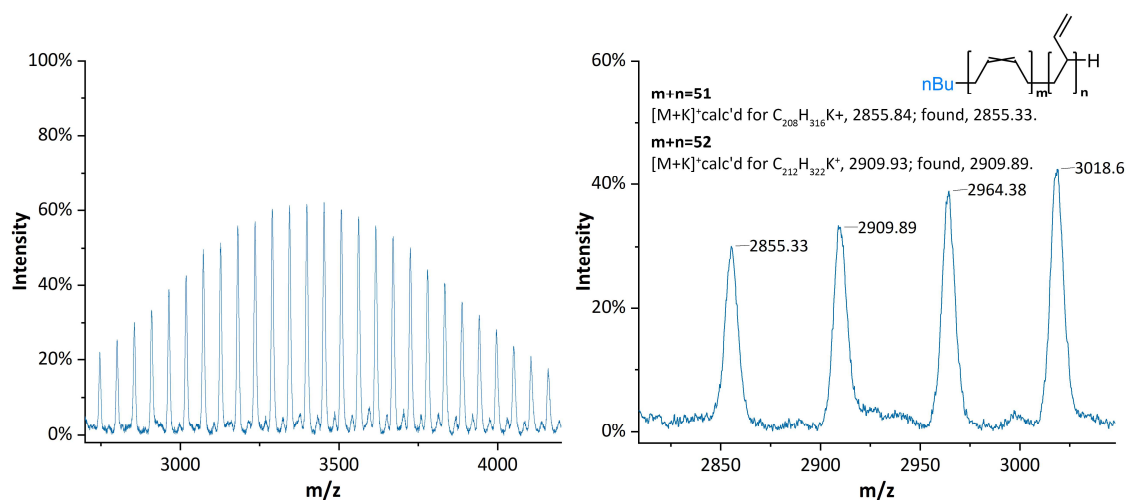


Figure S4. MALDI-TOF-MS spectrum of polybutadiene obtained using the n-BuLi/**6** DiPip initiator system.

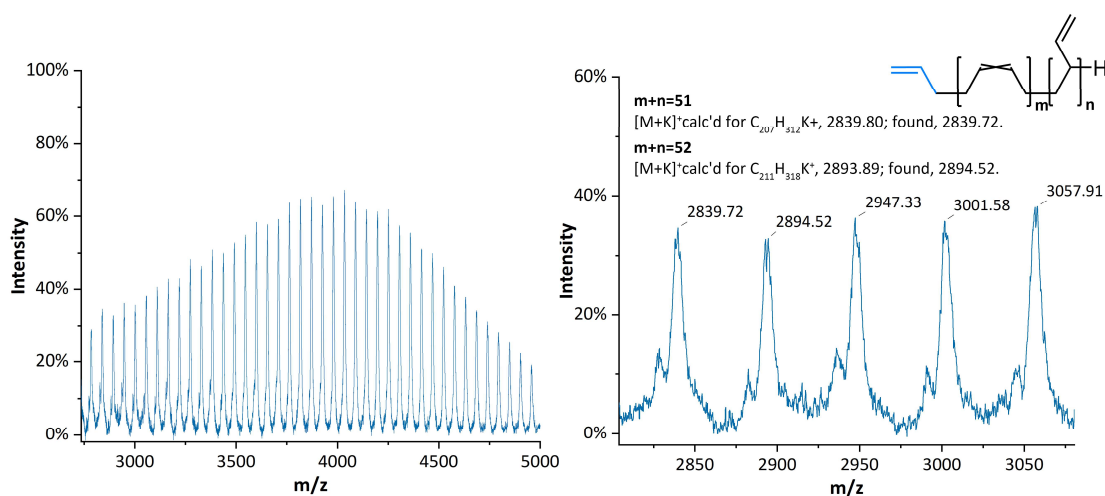


Figure S5. MALDI-TOF-MS spectrum of polybutadiene obtained using complex **6a** as the initiator.

MALDI-TOF-MS characterization was conducted on polybutadiene samples obtained using both the lithium complex **6a**, serving as a model for the active species, and the *n*-butyllithium/**6** DiPip initiator system. Due to the lower accuracy of MALDI-TOF-MS for high-molecular-weight polymers, we synthesized polymers with molecular weights in the range of 3000–4000 Da for this analysis. The resulting spectra are shown in Figures S4–S5. These spectra indicate that, regardless of the initiation system used, the molecular weight of each repeating unit is 54 Da, consistent with the structural unit of polybutadiene.

Molecular weight analysis, however, reveals distinct differences in the end-group structures depending on the initiation system. For the *n*-butyllithium/**6** DiPip system, assuming a butyl end-group and a degree of polymerization of 51, the structure $C_{208}H_{316}$ has a theoretical molecular weight of $[M+K]^+$ at 2855.84 Da, closely matching the experimental value of 2855.33 Da (Figure S4). For the polymer initiated by complex **6a**, assuming an allyl end-group and a polymerization degree of 51, the structure $C_{207}H_{312}$ has a theoretical molecular weight of $[M+K]^+$ at 2839.80 Da, in agreement with the experimental value of 2839.72 Da (Figure S5), thus confirming the expected end-group structures.

Complex **6a** was synthesized specifically as a model for the active species, polybutadienyllithium. The difference in end-groups between the two initiation systems is expected, as in a “living” polymerization without chain-transfer reactions, the initiator structure remains at the polymer chain end. This does not impact the validity of complex **6a** as a model compound for the active species. Our experiments confirm that complex **6a** exhibits initiating capability for “living” polymerization comparable to that of the *n*-butyllithium/**6** DiPip system. Moreover, NMR studies of the polymers obtained from both initiators demonstrate that they share the same microstructure, further supporting the reliability of complex **6a** as a model for polybutadienyllithium.

Quantitative Study of Lewis Base Steric Hindrance and Its Influence on 1,2-Selectivity in Initiator Systems Using Steric Maps

SambVca 2¹ is a quantitative analysis program for catalytic/initiator systems based on topological steric maps and has proven to be a powerful tool for analyzing the steric effects of complexes². The steric maps generated by this program allow for the calculation of the percent buried volumes (% VBur), a parameter that quantifies the volume occupied by ligands around a metal center². The primary application of the % VBur parameter is to guide the design of metal catalysts for a range of chemical reactions, as the steric environment surrounding the metal center can significantly impact both catalyst selectivity and activity. In summary, the % VBur parameter, developed by Cavallo and colleagues, has been shown to be instrumental in the development of new catalysts/initiators and is widely used to evaluate the relationship between steric hindrance and the activity/selectivity of polymerization catalysts³⁻⁵.

In this work, we propose a hypothesis of a strong correlation between the steric hindrance of Lewis bases and the regioselectivity of initiators, applying the “conformational constraint” theory to enhance the generalizability of this mechanism. To further support our proposed mechanism, we conducted quantitative and visual analyses of the steric maps and % VBur of active species models in the presence of Lewis bases using the SambVca 2 program. As shown in Figure S6a, the spatial constraints around the Li⁺ ion are more pronounced when **6** DiPip is used as the ligand compared to other Lewis bases. Additionally, there is a clear positive correlation between percent buried volumes and the 1,2-unit content in the resulting polymer. These analyses indicate that Lewis bases with higher % VBur provide greater steric hindrance, corresponding to polymers with a higher 1,2-unit content.

Figures S6b–d illustrate the effect of the “conformational constraint” on % VBur. It is evident that merely increasing the volume of the Lewis base does not enhance the “effective steric hindrance” at the active center, whereas increasing the rigidity of the ligand ring can significantly raise % VBur, thereby boosting the system’s 1,2-regioselectivity.

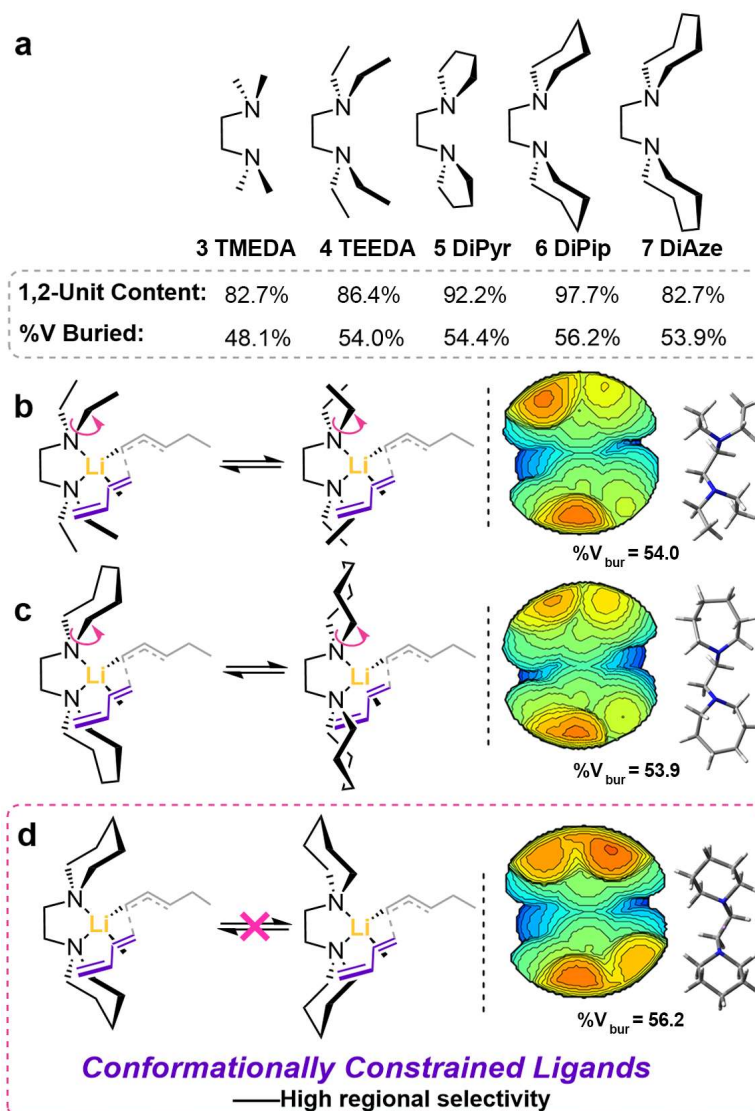


Figure S6. (a) Correlation between percent buried volumes of active species and 1,2-unit content in polybutadiene.

(b) and **(c)** Conformational flexibility in **4** TEEDA and **7** DiAze leading to reduced regioselectivity. **(d)** Enhanced regioselectivity in **6** DiPip due to conformational constraint effects.

General Procedures and Materials

Commercially sourced n-butyllithium and tert-butyllithium were stored at -36°C in a glove box and their concentrations were determined by titration analysis before use. Tetrahydrofuran (**2** THF), **1** glyme, N,N,N',N'-tetramethylethylenediamine (**3** TMEDA), and N,N,N',N'-tetraethylethylenediamine (**4** TEEDA) were all commercial reagents. They were purified under nitrogen protection by refluxing with sodium and subsequent distillation, and then stored in the glove box. n-Hexane, n-pentane, and benzene-*d*₆ were purified under nitrogen by refluxing with a Na/K alloy and benzophenone, followed by distillation

and storage with 4Å molecular sieves under nitrogen. They were degassed before use. Dichloromethane was dried using 3Å molecular sieves. THF-*d*₈ was dehydrated through 3Å molecular sieves, degassed, and stored in the glove box. Ethanol and deuterated methanol used for terminating the polymerization reactions were dehydrated through 3Å molecular sieves and oxygen was removed by freeze-pump-thaw cycling to prevent oxygen-induced coupling.

Characterizations

¹H NMR and ¹³C NMR spectra were recorded on a 500 MHz Bruker Avance NEO or a 400 MHz Bruker Avance III spectrometer, with HSQC spectra obtained via the 500 MHz system. These were reported relative to TMS or the residual solvent peak. The microstructure characterization of polybutadiene is primarily conducted via NMR. Specifically, the integrals of the peaks at 4.9 ppm and 5.4 ppm in the ¹H NMR spectrum are calculated, and the 1,2-unit content is determined using the following formula. According to the reported methods⁶, ¹³C NMR is used as an auxiliary tool to confirm the cis-trans ratio of the 1,4-units in the polymer.

$$1,2\text{-Unit}\% = \frac{I_{4.9}}{I_{5.4} + I_{(4.9/2)}}$$

²H NMR spectra were acquired using a 400 MHz Bruker Avance III, employing carbon tetrachloride as the solvent and a small amount of deuterated chloroform as an internal standard (7.26 ppm).

High-resolution mass spectra were recorded using a Waters ACQUITY UPLC H-Class/Xevo in line with a Waters Xevo G2 Q-TOF mass spectrometer.

The analysis of the average molecular weight and distribution of the polymers was conducted using an Agilent 1260 Infinity system equipped with an Agilent PLgel 5µm MIXED-C column and an Agilent 1260 Infinity refractive index detector. Polystyrene standards from Agilent were used as references. For the analysis of polybutadiene samples, calibration was performed through the universal calibration principle with Mark-Houwink equation parameters of $\alpha = 0.81$ and $K = 9.01 \times 10^{-5}$.⁷

The microstructure of the polybutadiene product was analyzed using ¹H NMR and ¹³C NMR, calculated using the formula reported by Forens et al.,⁸ and validated by FTIR.

FTIR spectra were obtained on a Bruker Tensor II FTIR spectrometer in ATR mode and reported in the frequency of absorption (cm⁻¹).

The MALDI-TOF-MS spectra were acquired using a Bruker Microflex LT mass spectrometer. Following an improved method reported by Frey et al.⁹, solutions of dithranol (20 mg/mL), polybutadiene (10 mg/mL), and silver trifluoroacetate (10 mg/mL) were prepared in tetrahydrofuran. These solutions were then thoroughly mixed in a 10:1:2 ratio, and approximately 1 µL of the mixture was quickly spotted onto the sample plate and dried at room temperature. The analysis was conducted in positive ion/linear mode.

Differential scanning calorimetry (DSC) measurements, including recording the DSC curves and determining the glass transition temperature (*T*_g) of the polymers, were performed using a Netzsch DSC204F1 calorimeter. Samples were prepared by precisely weighing approximately 5 mg of polymer and sealing it in an aluminum crucible. After removing thermal history, the samples were heated at a

rate of 10°C/min during the testing process.

Single-crystal X-ray diffraction data were collected using a Rigaku XtaLAB Synergy diffractometer. This device employs a graphite-monochromated Mo-K α radiation source, characterized by a wavelength of 0.71073 Å, and operated at a temperature of 100.00(10) K. Suitable crystals were selected, mounted, and sealed within Lindemann capillaries in a dry nitrogen environment. The data integrated with CrysAlisPro 1.171.42.84a (Rigaku Oxford Diffraction, 2023) and a multi-scan absorption correction using SCALE3 ABSPACK was applied. The structure elucidation of the Li complex was achieved through the Olex 2 software¹⁰, employing the SHELXT 2018/2 for initial solution and subsequently refining the structure based on F^2 using full-matrix least-squares methods via SHELXL 2018/3.¹¹ All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were refined isotropic on calculated positions using a riding model with their U_{iso} values constrained to 1.5 times the U_{eq} of their pivot atoms for terminal sp³ carbon atoms and 1.2 times for all other carbon atoms. Finally, the graphical representation of the thermal ellipsoid plot (ORTEP) was generated using the Ortep-3 software¹².

Typical Procedure for 1,3-Butadiene Polymerization

The polymerization of 1,3-butadiene was conducted in a 50 mL Schlenk tube equipped with a rubber stopper. All vessels and rubber stoppers were pre-dried in an oven or under vacuum before use. Under nitrogen protection, n-hexane, 1,3-butadiene, and the Lewis base were sequentially added to the polymerization system. After a standard purification process, t-butyllithium was introduced into the system using a syringe, followed by thorough mixing. The reaction was then allowed to proceed for 10 hours at 20°C. The reaction was terminated with 0.1 mL of degassed ethanol containing 1% BHT. The organic phase was washed three times with 2 M hydrochloric acid, retaining the organic phase, which was then poured into an excess of ethanol to precipitate the polymer. The polymer was vacuum-dried at 80°C to constant weight.

Synthesis of Selectively Deuterated Polybutadienyllithium for in-Situ NMR Testing

Synthesis of 2,2,5,5-tetradeuterated-3-sulfolene. Under a nitrogen atmosphere, 25 g of 3-sulfolene, 0.3 g of anhydrous potassium carbonate, 30 mL of dry 1,4-dioxane, and 50 mL of deuterium oxide (99.9% D) were added to a Schlenk flask. After stirring at room temperature for 24 hours, all solvents were removed by vacuum distillation. The flask was then refilled with 30 mL of dry 1,4-dioxane and 50 mL of fresh deuterium oxide, and the mixture was stirred again at room temperature for 24 hours, followed by the removal of volatiles under vacuum. This process was repeated a total of 5 times, ultimately yielding 1,1,4,4-tetradeuterobutadiene with a deuterium enrichment of over 99% (25.8 g, quantitative yield). Figure S7 shows the ¹H NMR spectra of 3-sulfolene sample after undergoing different numbers

of deuterium substitution reactions. ^1H NMR (500 MHz, chloroform- d) δ 6.08 – 6.00 (m, 2H).

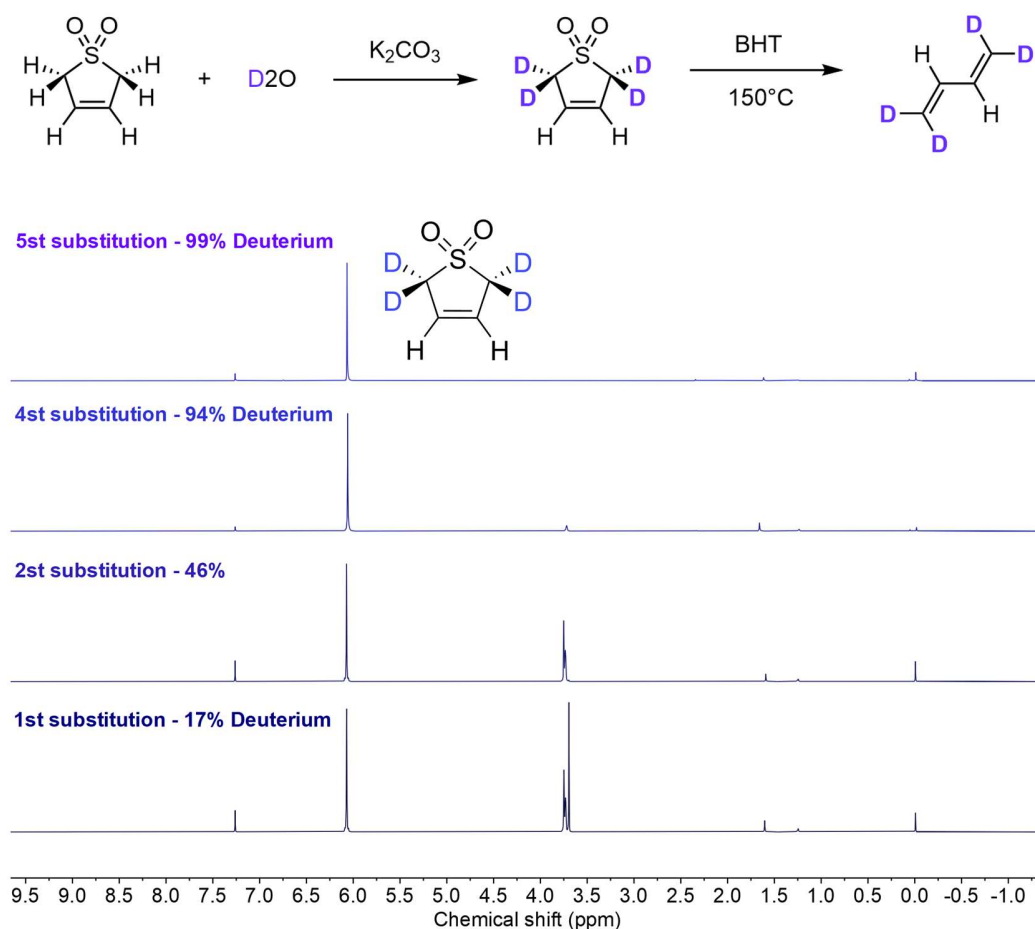


Figure S7. ^1H NMR spectra (400 MHz, in CDCl_3) of 3-sulfolene sample after undergoing different numbers of deuterium substitution reactions.

Synthesis of 1,1,4,4-tetradeuterobutadiene. Set up the apparatus as shown in Figure S8 for the pyrolysis of 3-sulfolene- d_4 . Under nitrogen protection, load 25 g of the 3-sulfolene- d_4 and 0.25 g of 2,6-bis(1,1-dimethylethyl)-4-methylphenol into a Schlenk flask and heat to 150°C . The 3-sulfolene- d_4 decomposes upon heating to produce butadiene- d_4 and SO_2 . The SO_2 is removed through two sodium hydroxide scrubbers, and the moisture in the gases is removed using a drying tube filled with 3A molecular sieves. The purified butadiene- d_4 is then collected in a cold trap at liquid nitrogen temperature. The entire setup is initially purged with nitrogen, and a continuous stream of nitrogen is maintained at the Schlenk flask to prevent the polymerization of the butadiene- d_4 at high temperatures. When gas production ceases, a small amount of calcium hydride is added to the cold trap. The butadiene- d_4 is then condensed into a pressure-resistant glass container at -30°C using a slightly heated cold trap, and stored in a glove box refrigerator at -36°C along with 3Å molecular sieves. The deuterium enrichment of over 99% is confirmed by ^1H NMR spectroscopy (Figure S9). ^1H NMR (500 MHz, chloroform- d) δ 6.35 (s, 1H).

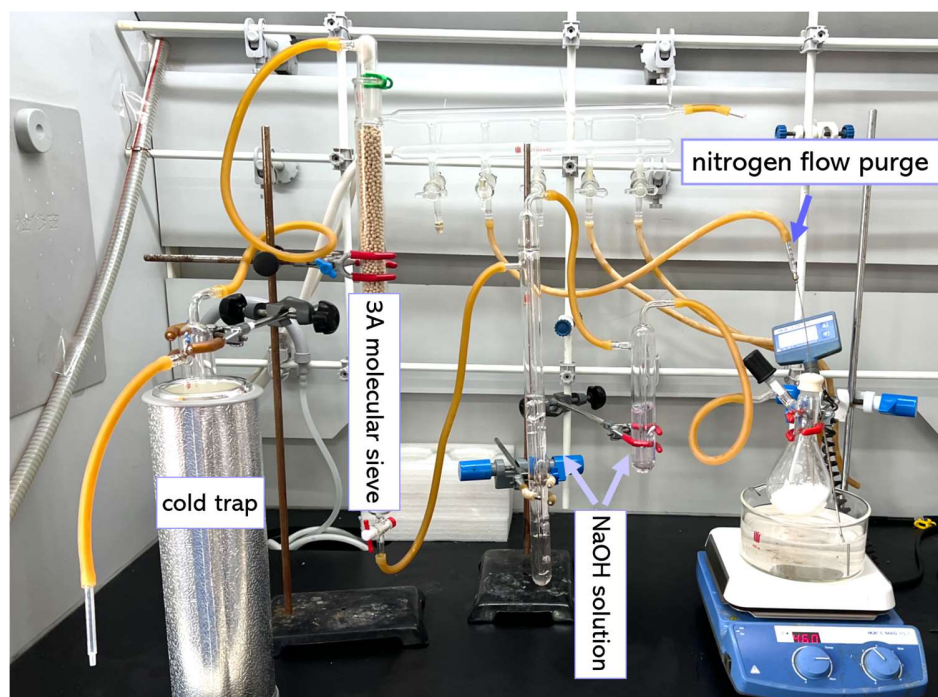


Figure S8. The apparatus for the pyrolysis of 3-sulfolene-d₄ to prepare 1,1,4,4-tetradeuterobutadiene.

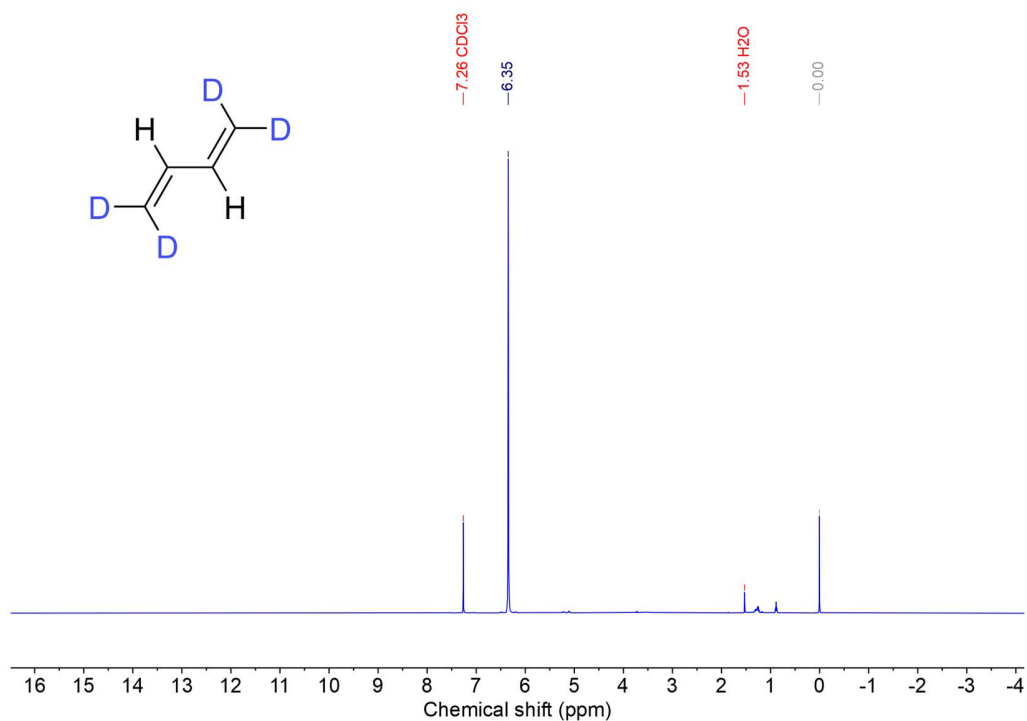
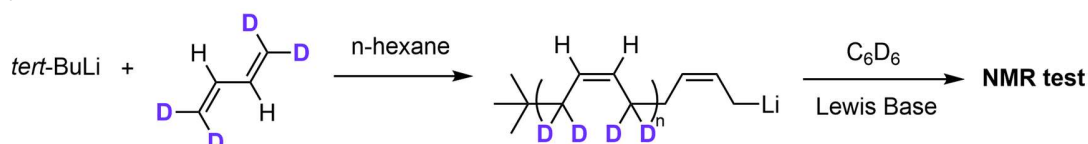


Figure S9. ¹H NMR spectrum of the 1,1,4,4-tetradeuterobutadiene (400 MHz, CDCl₃).

Preparation of selectively deuterated polybutadienyllithium for in-situ NMR testing. To eliminate the influence of the penultimate unit variation on the chain-end allyl's chemical shift and spin-spin coupling in NMR, we chose polybutadienyllithium with a 1,4-unit content of over 90% for the NMR experiments. By initiating polymerization in a very dilute solution in n-hexane, we successfully synthesized the target polymer. In a glove box filled with argon, 150 mL of n-hexane and 0.9 g of 1,1,4,4-tetradeuterobutadiene were added to a Schlenk flask. At room temperature, 1.3 mL of a solution of tert-butyllithium in pentane (1.3 M, 1.66 mmol) was added using a syringe. The mixture was shaken and left to react overnight at room temperature in the glove box. The solvent was removed under vacuum, and 10 mL of deuterated benzene was added, followed by the evaporation of the solvent again. This process was repeated three times to remove all n-hexane, yielding 0.9 g of a colorless, transparent, viscous oil. ^1H NMR analysis indicated that the polymer was polybutadienyllithium with 92% 1,4-unit content and an average polymerization degree of 9.4. It was dissolved in deuterated benzene, placed into a J. Young NMR tube, and different Lewis bases were added for in-situ NMR experiments.



Synthesis of Active Center Model 6a and Prepared for Single Crystals

Synthesis of $\text{Sn}(\text{allyl})_4$. (*Caution! Alkyltin compounds are highly neurotoxic and volatile.*) Tetraallyltin is prepared by reacting allylmagnesium bromide with tin tetrachloride¹³. We attempted to use commercially available allylmagnesium bromides from multiple sources, but their purity did not meet the requirements of our experiment, leading to the production of almost entirely triallyltin bromide. Only the allylmagnesium bromide prepared in-house succeeded in producing the desired product (see Figure S10). Therefore, following the method reported in the literature¹³, allylmagnesium bromide was prepared in ether using magnesium turnings and allyl bromide, and its concentration was determined by titration. Under nitrogen protection, 1100 mL of allylmagnesium bromide solution in ether (0.49 M, 539.0 mmol) was added to a Schlenk flask and cooled to -78°C . Under vigorous stirring, 17.3 g of pure SnCl_4 (53.9 mmol, 0.1 equivalent) was slowly added to the flask; do not attempt to dilute it. After the addition, the temperature was slowly raised to 0°C over 30 minutes and the reaction was maintained for another 30 minutes, then slowly brought to room temperature over 2 hours. The reaction was cooled to -35°C , quenched with 200 mL of saturated ammonium chloride solution, and stirred for over 30 minutes until the organic layer gradually clarified. The supernatant was carefully decanted, and the aqueous layer was washed and decanted three times with ether, combining the organic phases. The combined organic layer was dried over anhydrous sodium sulfate, filtered through diatomaceous earth, and the ether was evaporated under vacuum to

yield a colorless oily substance. This substance was washed four times with 5% potassium fluoride solution to remove triallyltin bromide until the potassium fluoride solution no longer turned cloudy. The organic layer was separated, dried over anhydrous sodium sulfate, filtered, and the ether was evaporated under vacuum. The product, tetraallyltin (7.2 g, 47% yield, boiling point: 95 Pa/63°C), was obtained as a colorless oily substance. Note: During the initial stages of vacuum distillation, continuous formation of low-boiling substances, possibly due to the decomposition of alkyltin ether complexes, hindered further reduction in vacuum. This phenomenon disappeared after about 1 hour. Care should be taken not to overheat during distillation and to minimize heating time, as the product gradually degrades at high temperatures. ¹H NMR (400 MHz, chloroform-d) δ 5.9 (ddt, *J* = 17.0, 10.1, 8.6 Hz, 4H), 4.9 – 4.7 (m, 8H), 1.9 (td, *J* = 31.4, 8.5 Hz, 8H). ¹³C NMR (101 MHz, chloroform-d) δ 136.6 (t, *J* = 24.3 Hz), 111.1 (t, *J* = 25.3 Hz), 16.1 (t, *J* = 129.3 Hz).

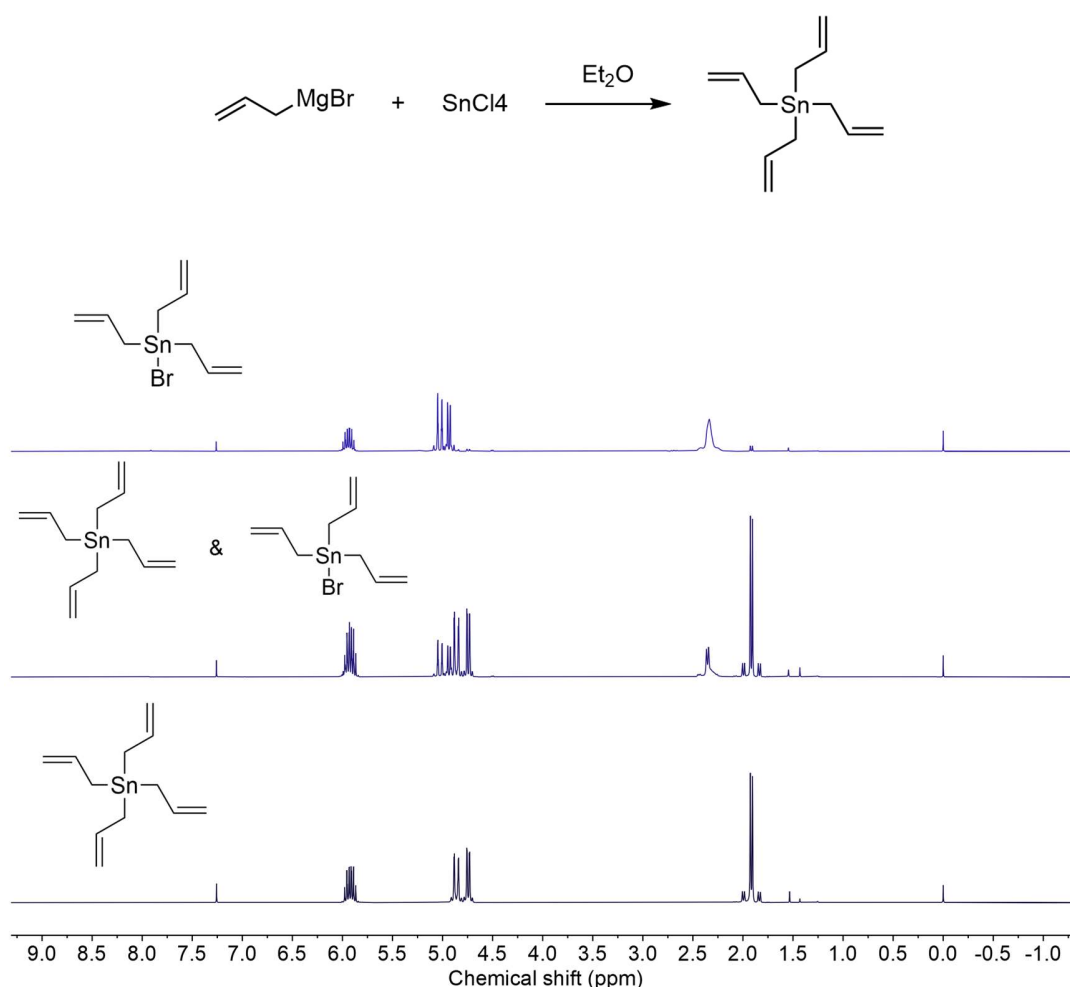
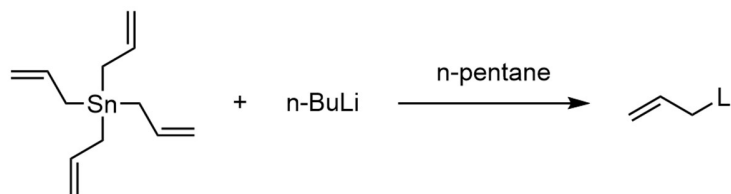


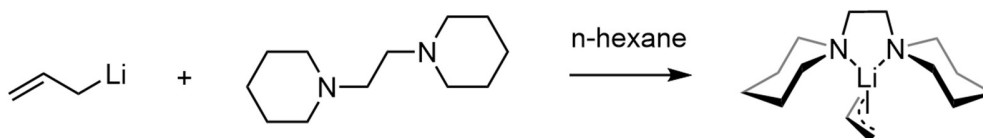
Figure S10. ¹H NMR spectra of tetraallyltin and triallyltin bromide (an impurity resulting from the use of commercial allylmagnesium bromide)

Synthesis of allyllithium. (**Caution!** Allyllithium will spontaneously ignite in the air, so please handle it in the glove box throughout the process. Please carefully quench small amounts of spilled product.) The

preparation of allyllithium is carried out via a transmetalation reaction between tetraallyltin and *n*-butyllithium in *n*-pentane. Both tetraallyltin and *n*-butyllithium are soluble in *n*-pentane, while the product, allyllithium, precipitates out in *n*-pentane. This allows for the convenient isolation of relatively pure solid allyllithium. In an argon-filled glove box, 3.0 g of tetraallyltin was dissolved in 35 mL of *n*-pentane. At room temperature, 17 mL of *n*-butyllithium solution (2.5 M, 42.4 mmol) was added in one go. The solution was stirred for about 1 hour using a glass magnetic stir bar. The product formed was a very fine powder that could easily pass through sintered glass, so it was rapidly filtered using a 0.2 μm PTFE microporous filter membrane and washed several times with *n*-pentane. The solid was dried under vacuum at a temperature below room temperature to yield 1.75 g of allyllithium (86% yield) as a fine white powder. It ignites violently in air but can be stored for several months without degradation at low temperatures (-36°C) in a glove box. It is insoluble in hydrocarbon solvents but dissolves readily in nonpolar solvents with a small addition of THF. Contrary to the phenomenon reported in literature reference 3, we did not observe a decrease in conversion rate when the ratio of *n*-butyllithium to tetraallyltin exceeded 1:2 in our experiments. Therefore, the employed molar ratio was set at Li:Sn = 4:1. ^1H NMR (500 MHz, Benzene- d_6 /THF- d_8) δ 7.07 (p, $J = 11.8$ Hz, 1H), 2.93 (d, $J = 11.6$ Hz, 4H). ^{13}C NMR (126 MHz, Benzene- d_6 /THF- d_8) δ 148.9, 53.0.



Synthesis of complex 6a. In a glove box, 100 mg of allyllithium (2.08 mmol) was weighed and added to 10 mL of *n*-hexane to form a suspension. At room temperature, 429.4 mg of **6** DiPip (2.19 mmol) was added and the mixture was shaken until it transformed from a milky suspension to a yellow clear solution. The solution was concentrated and then frozen overnight at -36°C , resulting in the precipitation of light-yellow transparent crystals weighing 225.2 mg (yield 44.3%). Single crystals suitable for X-ray single crystal diffraction were grown by slowly cooling in an *n*-hexane/toluene solvent. The product, **6a**, is highly sensitive to air and temperature and should be sealed and stored at low temperatures in the glove box. The product is unstable and will gradually decompose even in the glove box. ^1H NMR (500 MHz, Benzene- d_6) δ 7.09 (q, $J = 11.9$ Hz, 1H), 3.08 (d, $J = 11.9$ Hz, 4H), 1.94 (s, 4H), 1.43 – 1.72 (br, 8H), 1.31 – 1.10 (br, 4H), 0.78 – 2.80 (br, overlapped). ^{13}C NMR (126 MHz, Benzene- d_6) δ 146.94, 128.35, 55.96, 55.92, 51.81, 25.13, 24.16.



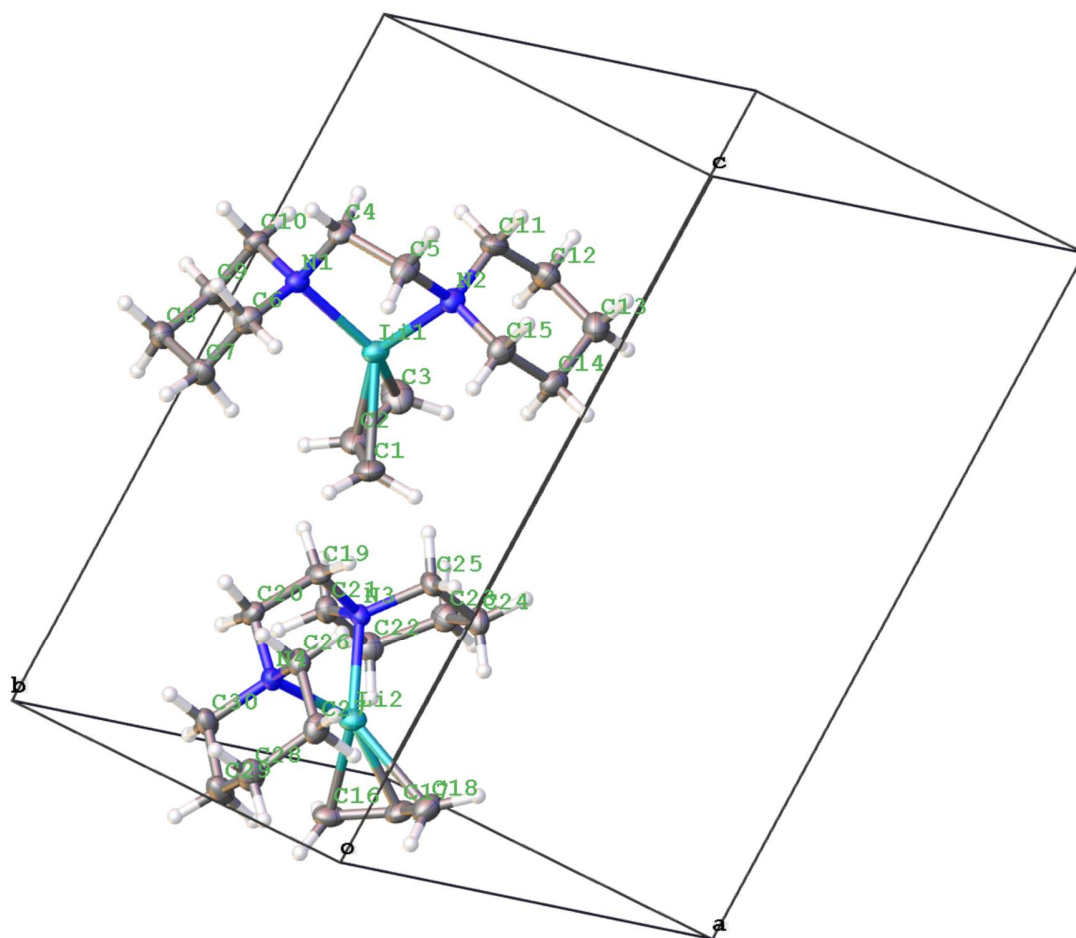


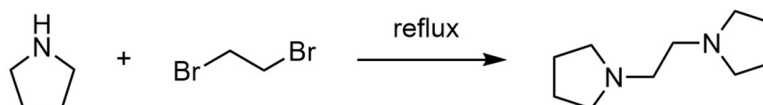
Figure S11. X-ray structure of complex **6a** with thermal ellipsoids at 50% probability.

Table S2. Crystal data and structure refinement of complex **6a**.

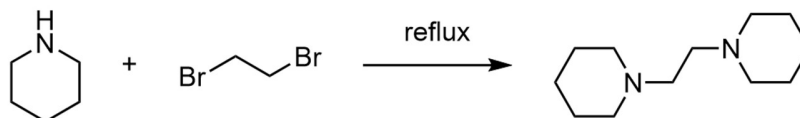
entry	data
empirical formula	C ₁₅ H ₂₉ LiIN ₂
formula weight	244.34
temperature (K)	100.00(10)
crystal system	triclinic
space group	$P\bar{1}$ (2)
<i>a</i> (Å)	8.9379(3)
<i>b</i> (Å)	12.3047(4)
<i>c</i> (Å)	14.7566(5)
α (°)	89.051(3)
β (°)	74.903(3)
γ (°)	86.783(3)
volume (Å ³)	1564.42(9)
<i>Z</i>	4
$\rho_{\text{calcd.}}$ (Mg m ⁻³)	1.037
μ (mm ⁻¹)	0.059
<i>F</i> (000)	544
crystal size (mm)	0.15×0.12×0.1
crystal colour	yellow
crystal shape	block
radiation	Mo <i>K</i> α (λ =0.71073 Å)
2 θ range (°)	4.37 to 62.05 (0.69 Å)
index ranges	−10 ≤ <i>h</i> ≤ 12 −15 ≤ <i>k</i> ≤ 16 −20 ≤ <i>l</i> ≤ 16
reflections collected	15299
independent reflections	7137 $R_{\text{int}} = 0.0273$ $R_{\text{sigma}} = 0.0340$
data/restraints/parameters	7137/2/325
Absorption correction	0.50730/1.00000
Tmin/Tmax (method)	(multi-scan)
goodness-of-fit on <i>F</i> ²	1.034
final <i>R</i> indexes [<i>I</i> ≥ 2 σ (<i>I</i>)]	<i>R</i> 1 = 0.0728, 0.1920
final <i>R</i> indexes [all data]	<i>R</i> 1 = 0.0896, <i>wR</i> ₂ = 0.2026
largest diff. peak and hole (e ^o Å ⁻³)	0.68/−0.70

Synthesis of the Lewis Base

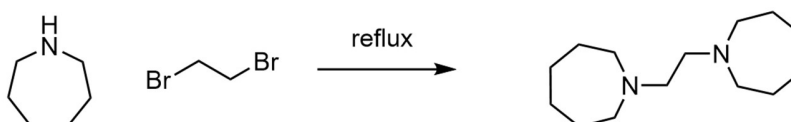
Synthesis of 1,2-dipyrrolidinoethane 5. In a 250 mL round-bottom flask, 20.0 g of pyrrolidine (281.2 mmol) and 13.2 g of 1,2-dibromoethane (70.3 mmol) were added, along with 100 mL of tetrahydrofuran (THF). The mixture was refluxed with stirring for 4 hours. After cooling slightly, the solvent was removed by vacuum evaporation. The product was then obtained through vacuum distillation, yielding 8.9 g (75% yield) of a colorless oily liquid. The boiling point of the product was about 49°C at 41 Pa. $^1\text{H NMR}$ (500 MHz, chloroform- d) δ 2.63 (s, 4H), 2.59 – 2.49 (m, 8H), 1.83 – 1.72 (m, 8H). $^{13}\text{C NMR}$ (126 MHz, chloroform- d) δ 55.7, 54.5, 23.4. **HRMS** (ESI/Q-TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{10}\text{H}_{21}\text{N}_2$ 169.1705; Found 169.1695.



Synthesis of 1,2-dipiperidinoethane 6. In a 250 mL round-bottom flask, 100 mL of tetrahydrofuran (THF), 25.0 g of piperidine (293.6 mmol) and 13.79 g of 1,2-dibromoethane (73.4 mmol) were added. The mixture was refluxed with stirring for 4 hours, followed by the removal of the solvent via vacuum evaporation. The product was then obtained through vacuum distillation, yielding 11.2 g (77% yield) of a colorless oil. The boiling point of the product was about 87°C at 75 Pa. $^1\text{H NMR}$ (500 MHz, chloroform- d) δ 2.48 (s, 4H), 2.40 (s, 8H), 1.57 (p, J = 5.6 Hz, 8H), 1.46 – 1.39 (m, 4H). $^{13}\text{C NMR}$ (126 MHz, chloroform- d) δ 56.8, 55.1, 26.0, 24.4.

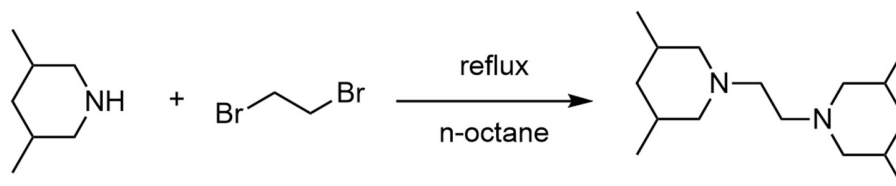


Synthesis of 1,2-dipiperidinoethane 7. In a 250 mL round-bottom flask, 25.0 g of piperidine (252.1 mmol) and 11.84 g of 1,2-dibromoethane (63.0 mmol) were added. The mixture was refluxed with stirring for 4 hours, followed by the removal of the solvent via vacuum evaporation. The product was then obtained through vacuum distillation, yielding 8.9 g (63.6% yield) of a colorless oily liquid. The boiling point of the product was 100°C at 81 Pa. $^1\text{H NMR}$ (400 MHz, chloroform- d) δ 2.70 – 2.63 (m, 8H), 2.62 (s, 4H), 1.68 – 1.55 (m, 16H). $^{13}\text{C NMR}$ (126 MHz, chloroform- d) δ 55.99, 55.96, 28.0, 27.0. **HRMS** (ESI/Q-TOF) m/z : $[\text{M} + \text{H}]^+$ Calcd for $\text{C}_{14}\text{H}_{29}\text{N}_2$ 225.2331; Found 225.2323.

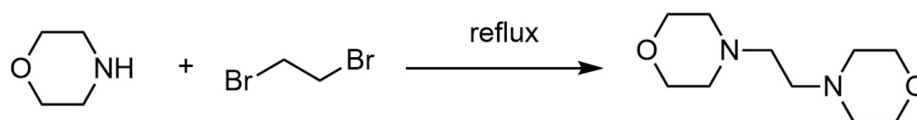


Synthesis of 1,2-bis(3,5-dimethylpiperidin-1-yl)ethane 8. In a 500 mL round-bottom flask, 200 mL of *n*-octane and 79.54 g of 3,5-dimethylpiperidine (isomer mixture, 702.64 mmol) are added. Then, 30.00 g of 1,2-dibromoethane (159.69 mmol) is slowly added dropwise at 120°C, during which a large amount

of white solid gradually forms. The mixture is stirred and refluxed for 6 hours, then cooled to room temperature. The solid is removed by filtration, and the solvent is removed by vacuum evaporation. Finally, the product is obtained by vacuum distillation, yielding 36.2 g (89.8%) of a colorless oily liquid. The product has a boiling point of 104°C at 104 Pa. $^1\text{H NMR}$ (500 MHz, chloroform- d) δ 2.83 (m), 2.50 (s), 2.48 – 2.26 (m), 2.07 (s), 1.87 (pd, J = 6.3, 3.6 Hz, 1H), 1.75 – 1.60 (m), 1.54 – 1.39 (m), 1.25 (t, J = 5.8 Hz), 0.93 (d, J = 6.8 Hz), 0.84 (d, J = 6.6, 1.6 Hz), 0.50 (m, J = 12.2, 10.7, 2.4 Hz). $^{13}\text{C NMR}$ (126 MHz, chloroform- d) δ 62.39, 62.26, 62.15, 61.71, 56.88, 56.35, 56.27, 42.21, 42.19, 39.14, 31.15, 31.11, 27.46, 19.71, 19.69, 19.24.

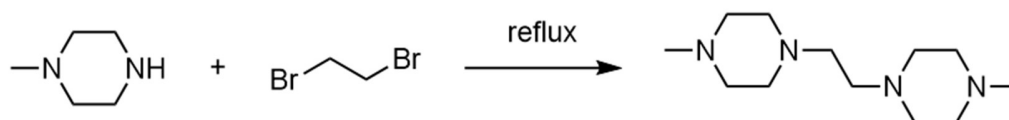


Synthesis of 1,2-dimorpholinoethane 9. In a 250 mL round-bottom flask, 70.00 g of morpholine (803.47 mmol) is added. The mixture is heated to 115°C, and 35.94 g of 1,2-dibromoethane (191.30 mmol) is slowly added dropwise with vigorous stirring. Significant exotherm is observed during the addition, so the dropwise addition rate should be controlled to prevent the solution from exceeding 120°C. After the addition is complete, the mixture is reacted overnight at 115°C, resulting in a large amount of solid. The reaction mixture is cooled to room temperature, ground with a mortar and pestle, and then continuously extracted three times with petroleum ether. The organic phase is filtered and retained. The solvent is removed from the organic phase by vacuum evaporation, yielding a large amount of solid. The product is purified by recrystallization from hot ethanol, resulting in 28.3 g (73.9%) of a colorless crystalline solid. $^1\text{H NMR}$ (500 MHz, chloroform- d) δ 3.74 – 3.66 (m, 8H), 2.52 (s, 4H), 2.49 (t, J = 4.9 Hz, 8H). $^{13}\text{C NMR}$ (126 MHz, chloroform- d) δ 66.96, 56.17, 54.17.

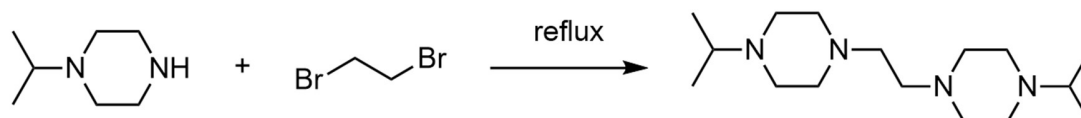


Synthesis of 1,2-bis(4-methylpiperazin-1-yl)ethane 10. In a 250 mL round-bottom flask, 70.00 g of N-methylpiperazine (698.85 mmol) is added. The mixture is heated to 115°C and 31.26 g of 1,2-dibromoethane (166.39 mmol) is slowly added dropwise with vigorous stirring. During the addition, significant exotherm is observed and the solution turns brown. It is necessary to control the addition rate to prevent the solution from exceeding 125°C. After the addition is complete, the mixture is heated overnight at 110°C, resulting in a large amount of solid. The reaction mixture is cooled to room temperature, ground with a mortar and pestle, and then continuously extracted three times with petroleum ether. The organic phase is filtered and retained. The solvent is removed from the organic phase by vacuum evaporation, and the product is purified by vacuum distillation, yielding 18.5 g (49.1%) of a colorless oily liquid. The product has a boiling point of 112°C at 98 Pa. $^1\text{H NMR}$ (500 MHz,

chloroform-d) δ 2.53 (s, overlapped), 1.88 – 3.14 (br, 26H), 2.28 (s, 6H). ^{13}C NMR (126 MHz, chloroform-d) δ 55.95, 55.14, 53.68, 46.08.



Synthesis of 1,2-bis(4-isopropylpiperazin-1-yl)ethane 11. In a 250 mL round-bottom flask, 50.00 g of N-isopropylpiperazine (391.24 mmol) is added. The mixture is heated to 115°C and 17.50 g of 1,2-dibromoethane (93.15 mmol) is slowly added dropwise with vigorous stirring. During the addition, significant exotherm is observed and the solution turns brown. It is necessary to control the addition rate to prevent the solution from exceeding 125°C. After the addition is complete, the mixture is heated overnight at 110°C, resulting in a large amount of solid. The reaction mixture is cooled to room temperature, ground with a mortar and pestle, and then continuously extracted three times with petroleum ether. The organic phase is filtered and retained. The solvent is removed from the organic phase by vacuum evaporation, and the product is purified by vacuum distillation, yielding 11.3 g (42.9%) of a colorless oily liquid. The product has a boiling point of 136°C at 93 Pa. ^1H NMR (500 MHz, chloroform-d) δ 3.15 – 1.86 (br m, 22H), 1.02 (d, J = 6.6 Hz, 12H). ^{13}C NMR (126 MHz, chloroform-d) δ 55.96, 54.38, 54.03, 48.64, 18.65.



Computational Details

The DFT calculations were conducted using Gaussian 09¹⁴ and OCRA 5.0.3^{15, 16} programs. We optimized and identified stationary points as either energy minima ($N_{\text{imag}} = 0$) or transition states ($N_{\text{imag}} = 1$) using the B3LYP¹⁷/6-31+G(d,p) level. To accurately account for the van der Waals interactions, a dispersion correction was applied, specifically the Grimme's D3 version of the Becke-Johnson damping (GD3BJ) method¹⁸. This approach has been shown to significantly improve the description of non-covalent interactions in molecular systems. Transition states were determined through the TS (berny) or QTS2 method, ensuring each corresponded to a single imaginary frequency along the reaction coordinate, as verified by frequency analysis. The intrinsic reaction coordinate (IRC) was employed to confirm the connectivity of each transition state¹⁹.

For more accurate relative energies, the single-point energy were calculated on the optimized structures at the $\omega\text{B97X-2-D3(BJ)}^{20, 21}/\text{def2-QZVPP}$ level with OCRA 5.0.3, incorporating solvation effects via the Universal Solvation Model Based on Solute Electron Density (SMD)²². As a double-hybrid density functional, $\omega\text{B97X-2-D3(BJ)}$ offers high accuracy and robustness, proven to be highly suitable for precision computational tasks in organic and organometallic systems. In combination with the high-precision 4-zeta basis set def2-QZVPP, it provides assurance for accurately comparing single-point

energies and energy barrier differences.

Unless specified, free energies (ΔG , 298.15 K, 1 atm) in solutions for energy profile descriptions were derived from solvation single-point calculations and gas-phase Gibbs free-energy corrections.²³ Acknowledging potential overestimations of entropy contributions to free energy in the ideal gas model, we applied Martin et al.'s method for minimizing error, namely a standard condition correction of 4.3 kcal/mol for each component change in each reaction²⁴.

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Spectroscopic Data — NMR Spectra of Lewis Bases and Intermediates

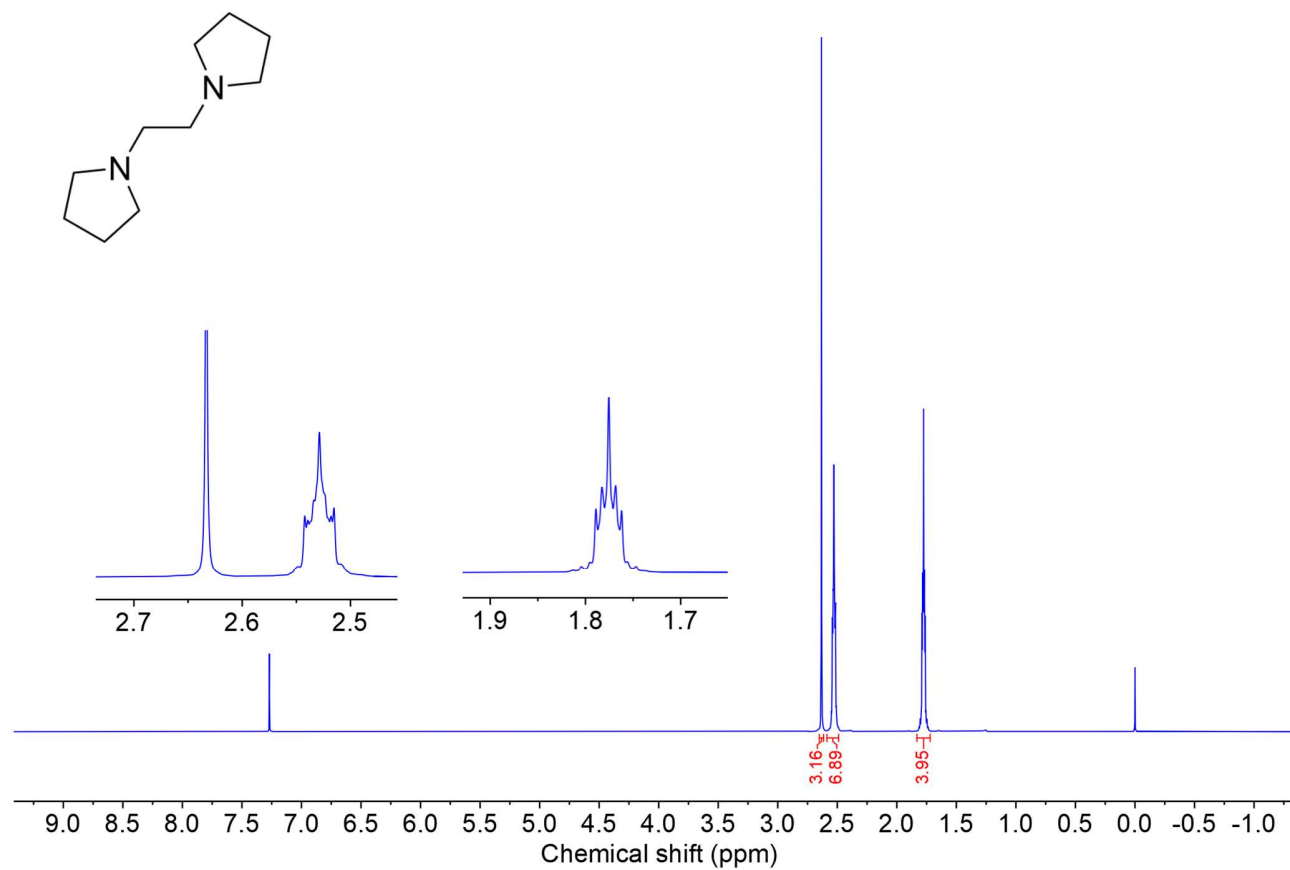


Figure S12. ^1H NMR spectrum of 1,2-dipyrrolidinoethane **5** (500 MHz, CDCl_3).

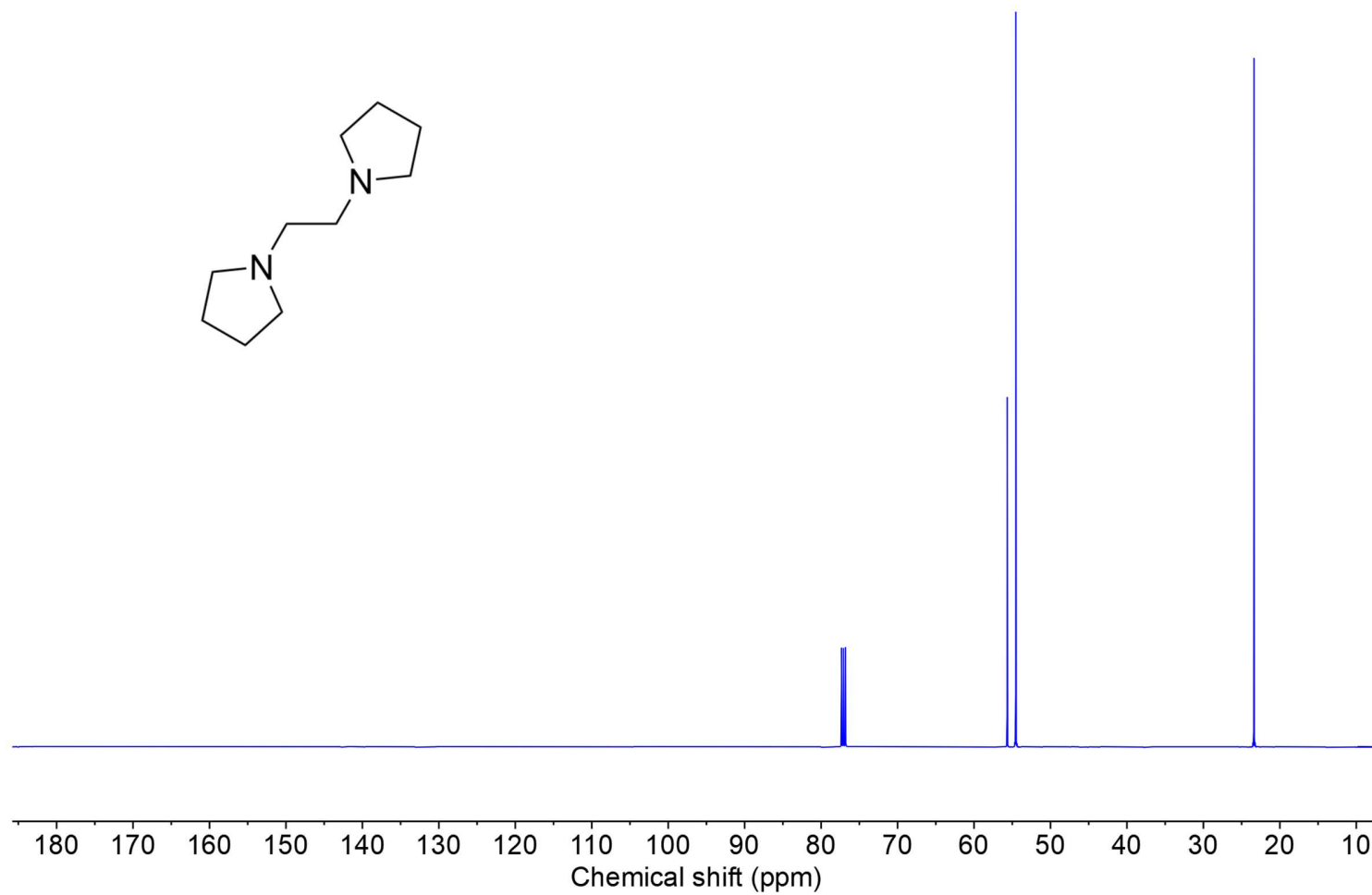


Figure S13. ^{13}C NMR spectrum of 1,2-dipyrrolidinoethane **5** (126 MHz, CDCl_3).

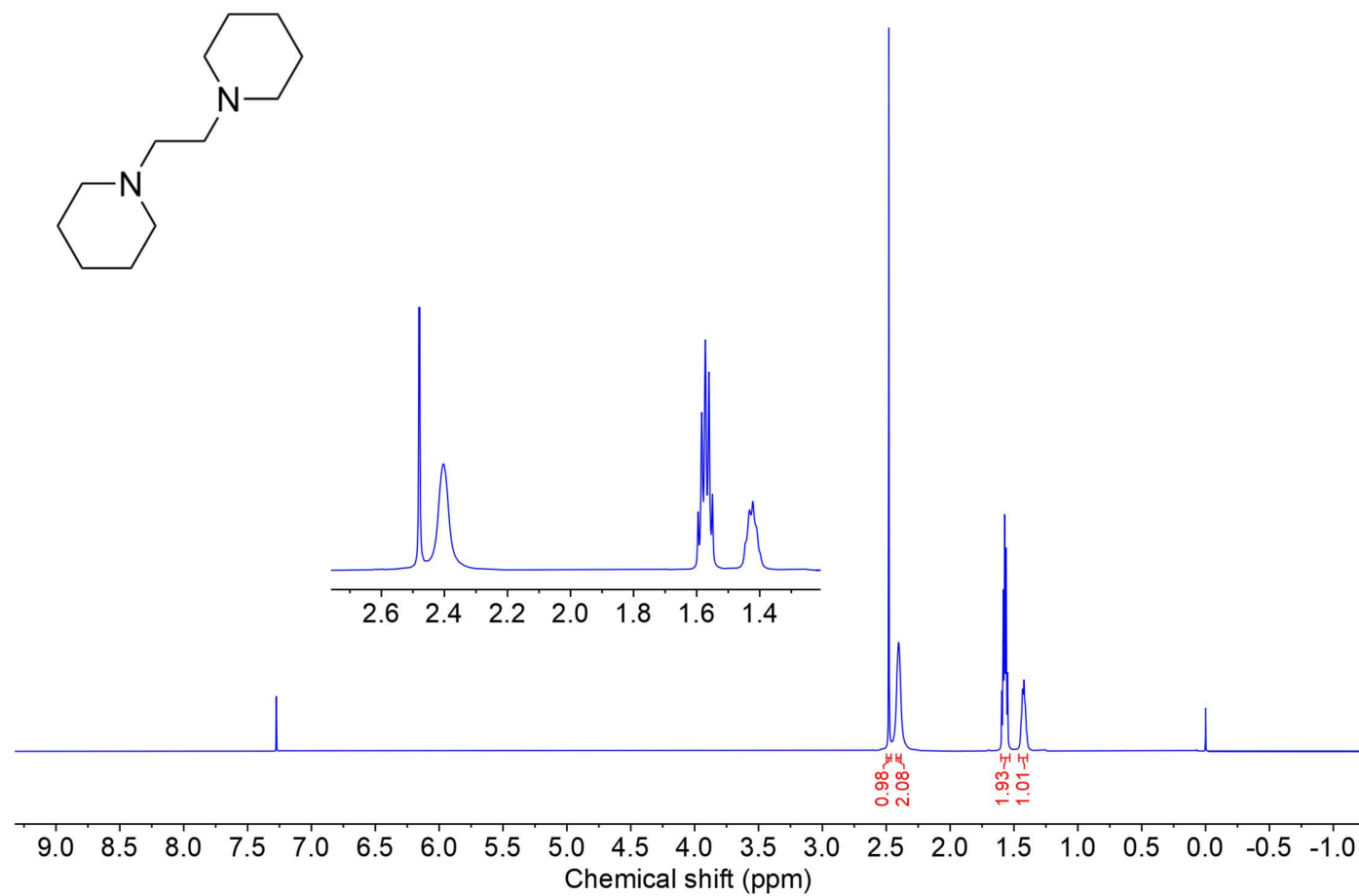


Figure S14. ^1H NMR spectrum of 1,2-dipiperidinoethane **6** (500 MHz, CDCl_3).

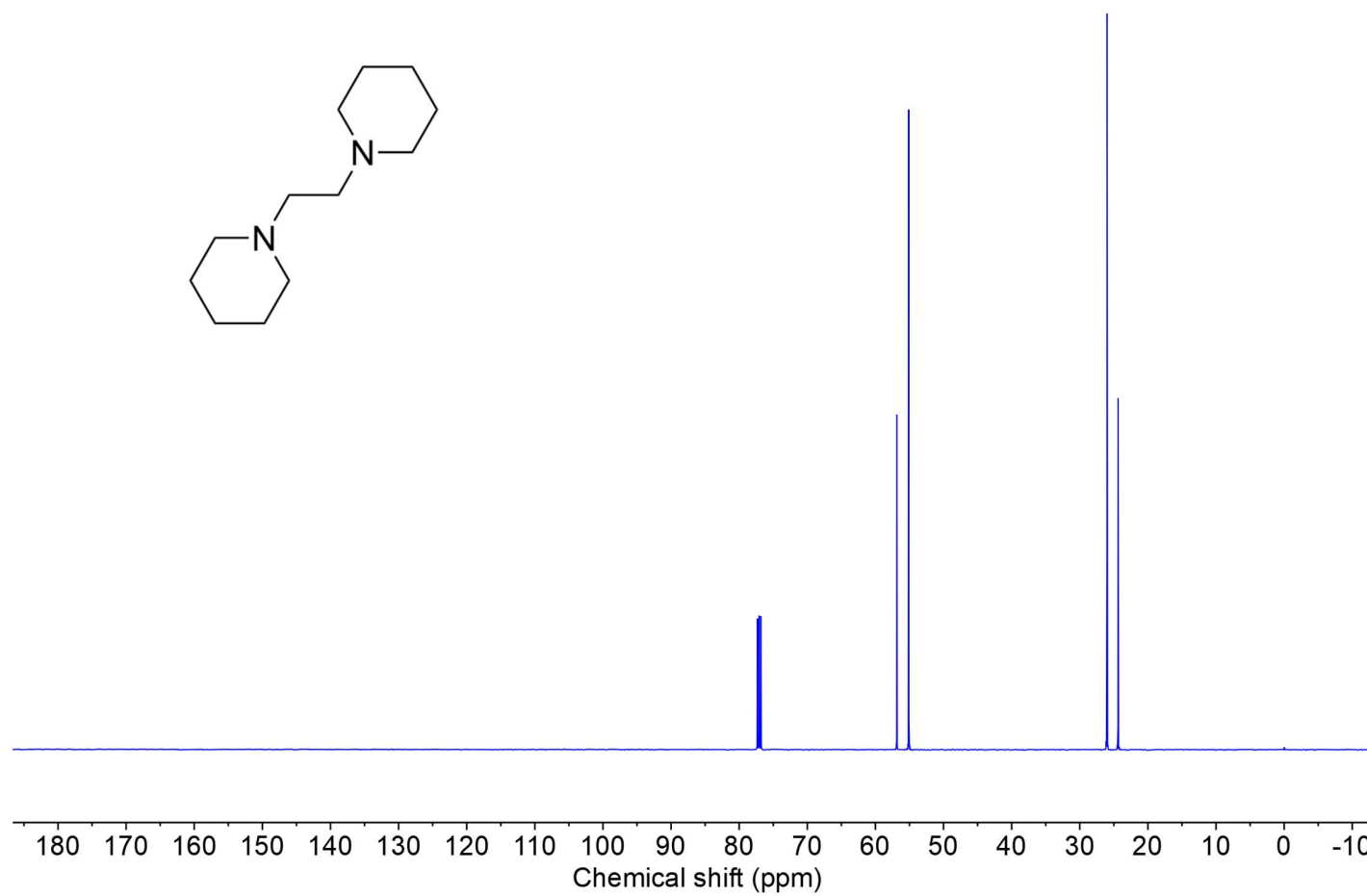


Figure S15. ^{13}C NMR spectrum of 1,2-dipiperidinoethane **6** (126 MHz, chloroform-d).

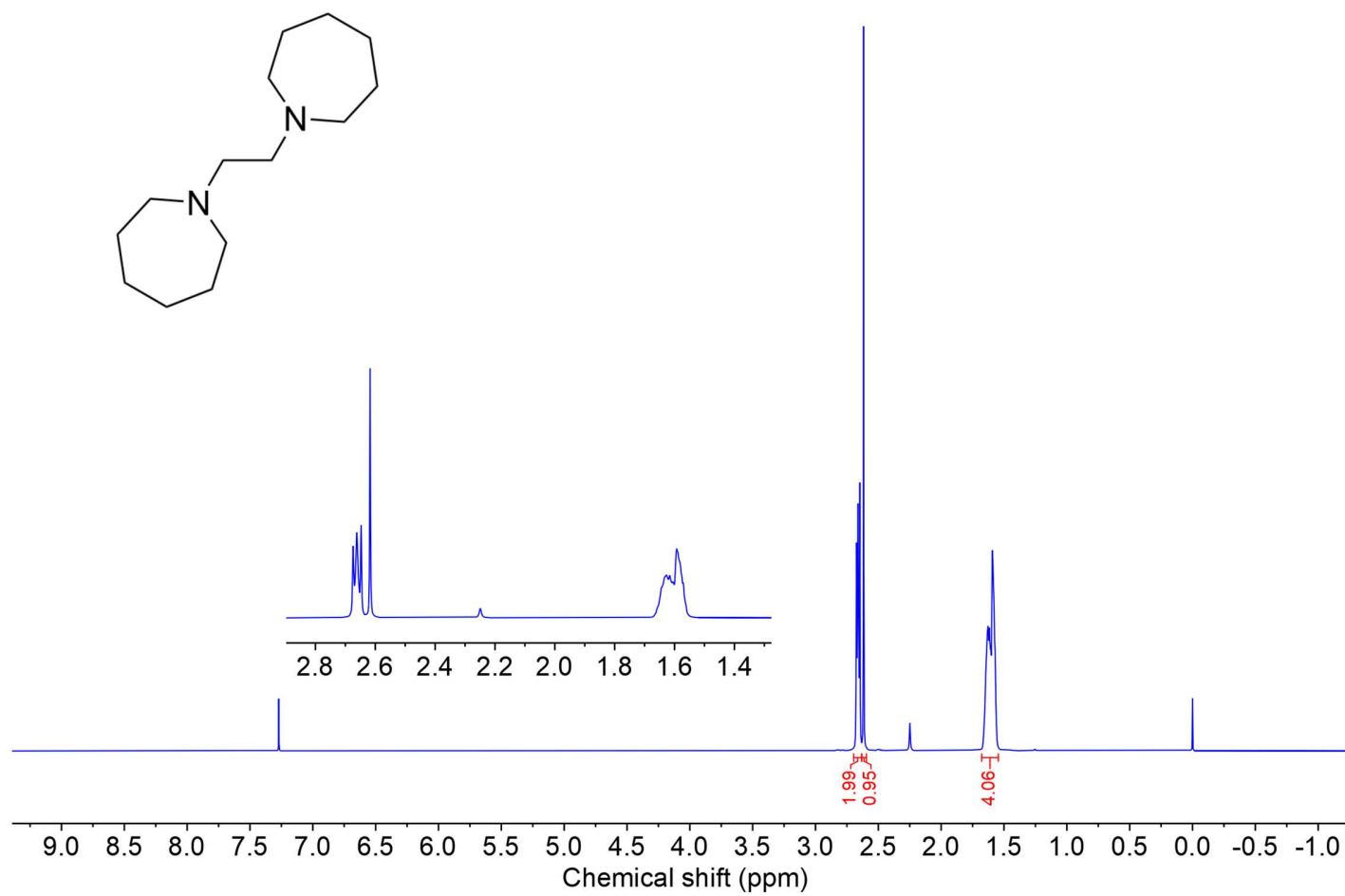


Figure S16. ^1H NMR spectrum of 1,2-dipiperidinoethane **7** (500 MHz, chloroform-d).

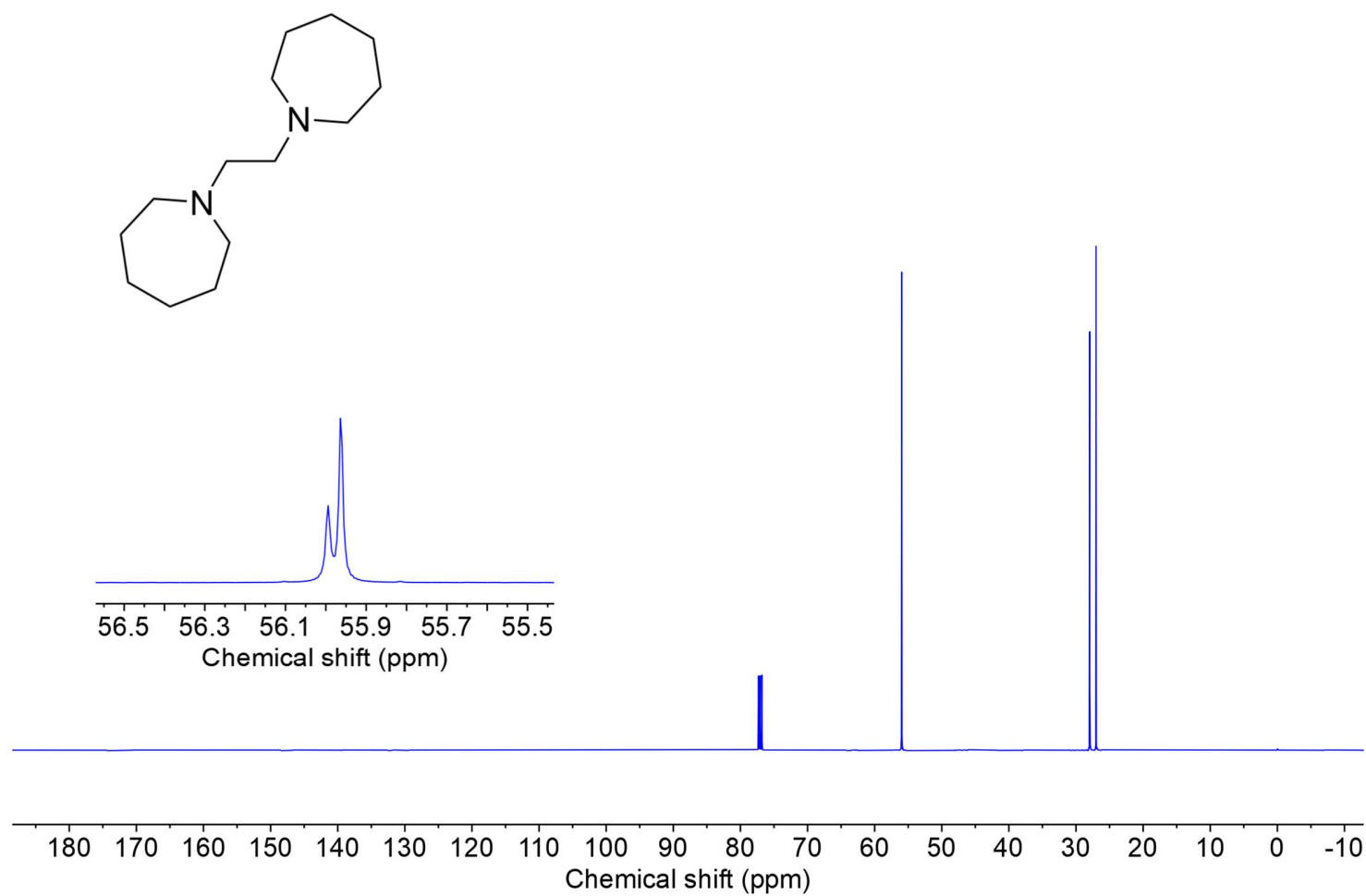


Figure S17. ^{13}C NMR spectrum of 1,2-dipiperidinoethane **7** (126 MHz, chloroform-d).

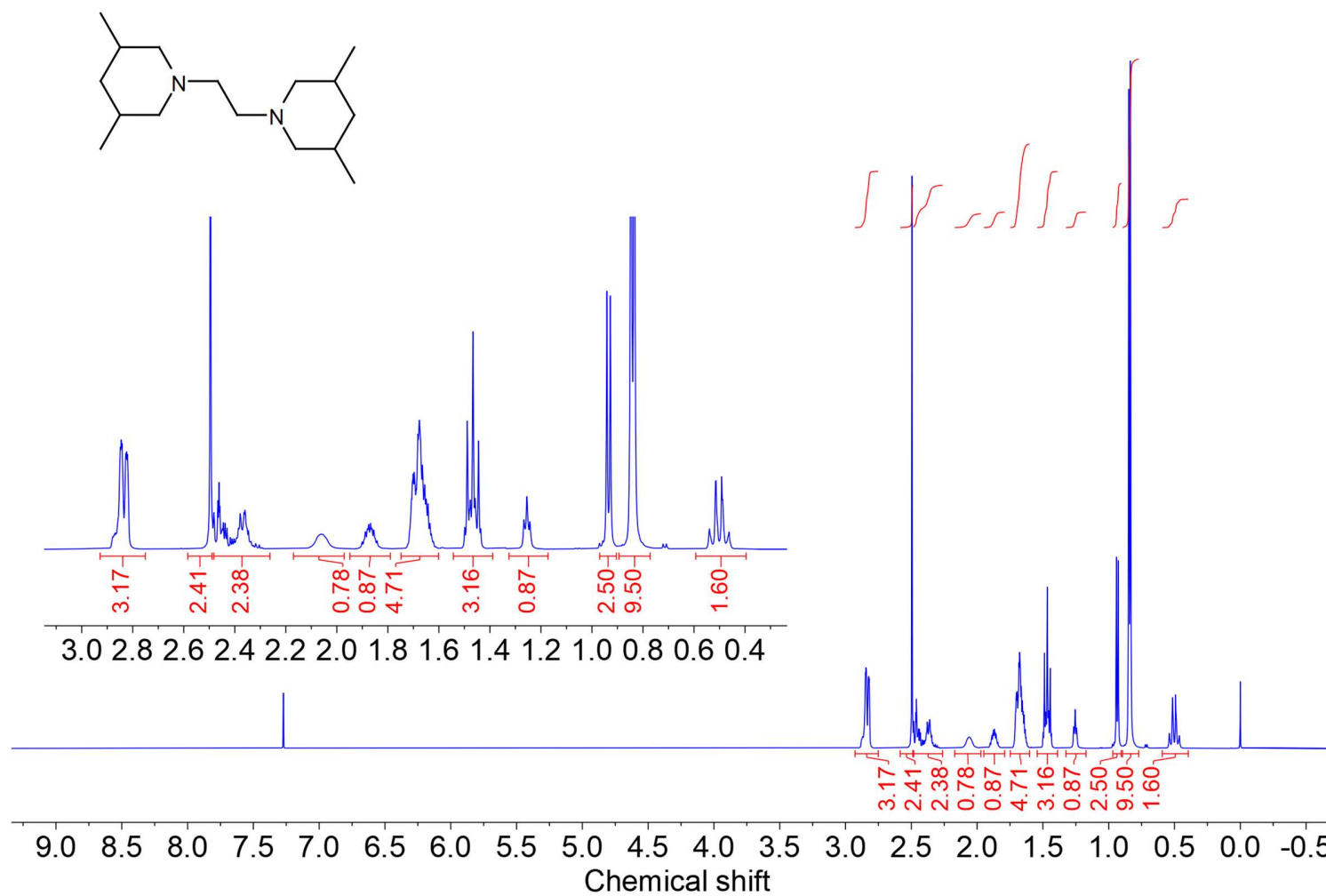


Figure S18. ^1H NMR spectrum of 1,2-bis(3,5-dimethylpiperidin-1-yl)ethane **8** (500 MHz, CDCl_3).

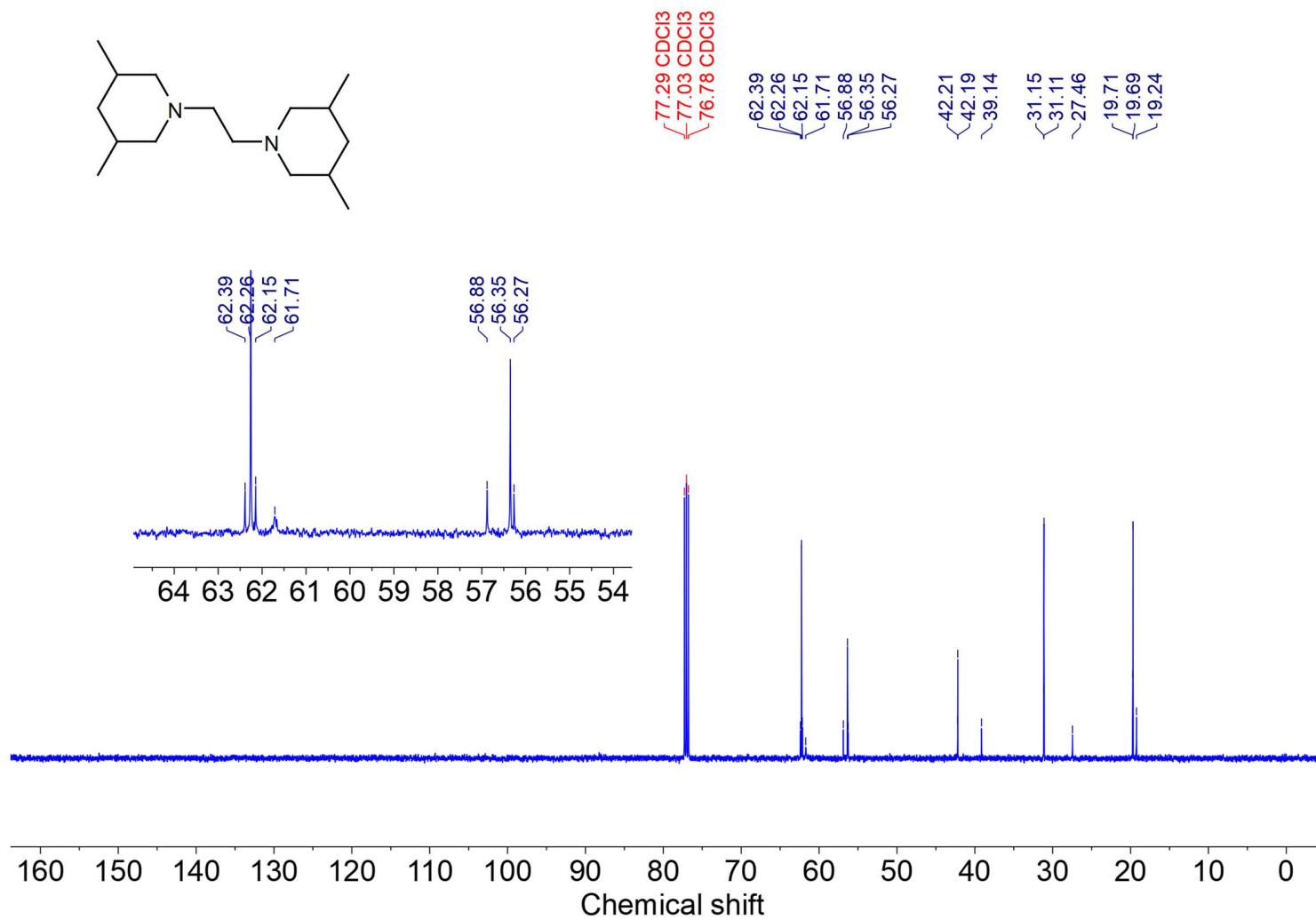


Figure S19. ^{13}C NMR spectrum of 1,2-bis(3,5-dimethylpiperidin-1-yl)ethane **8** (126 MHz, chloroform-d).

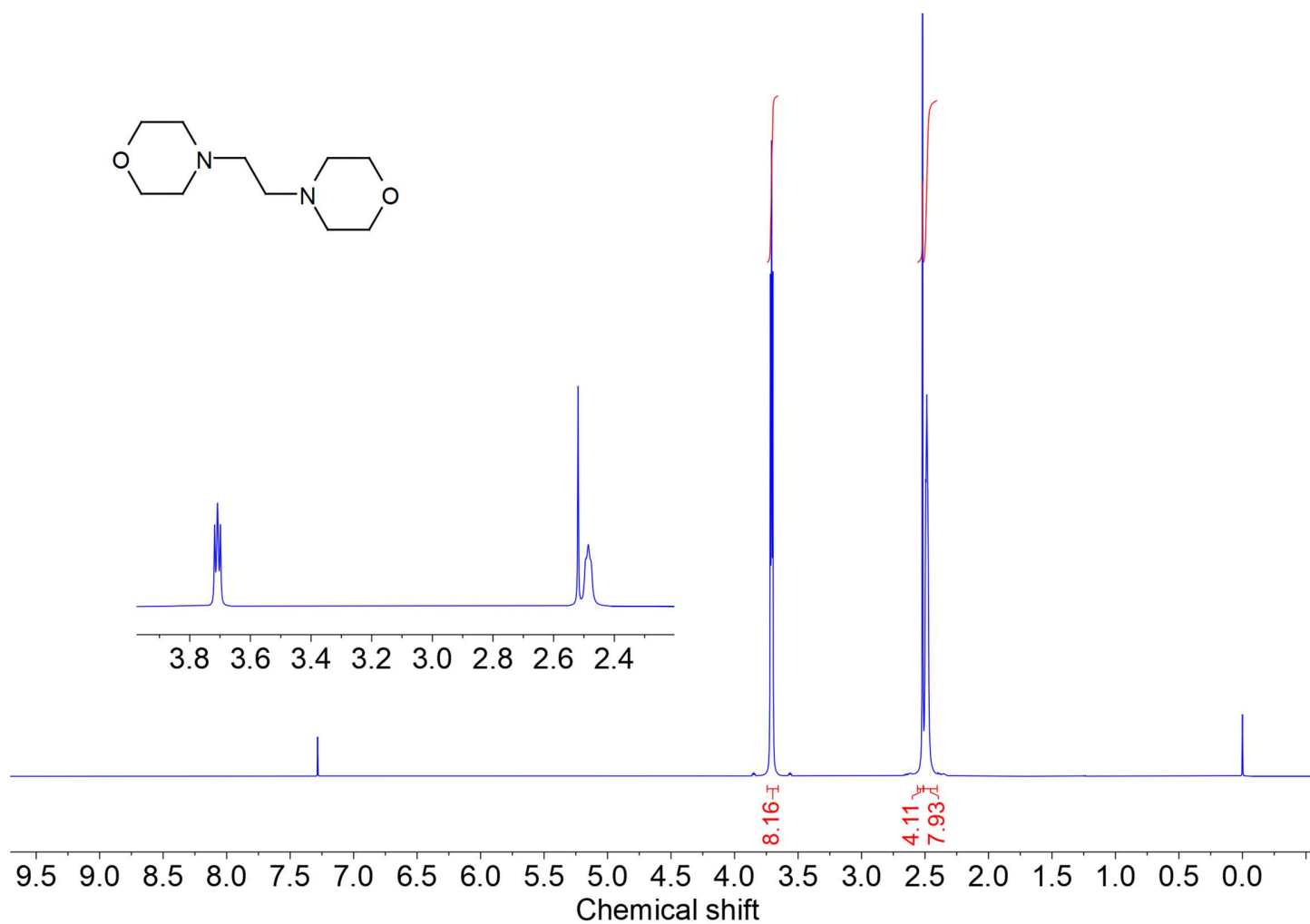


Figure S20. ¹H NMR spectrum of 1,2-dimorpholinoethane **9** (500 MHz, chloroform-d).

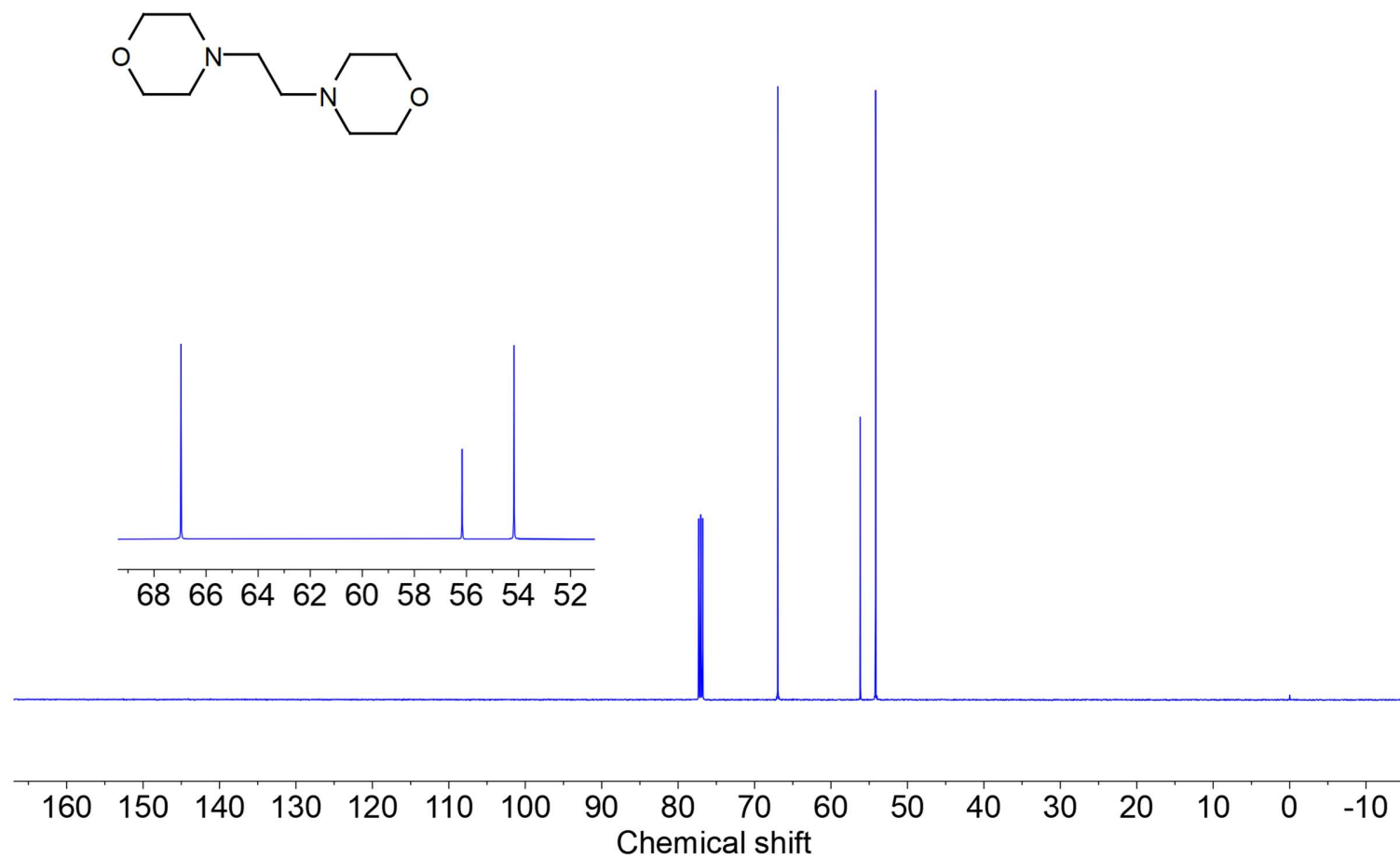


Figure S21. ¹³C NMR spectrum of 1,2-dimorpholinoethane **9** (126 MHz, chloroform-d).

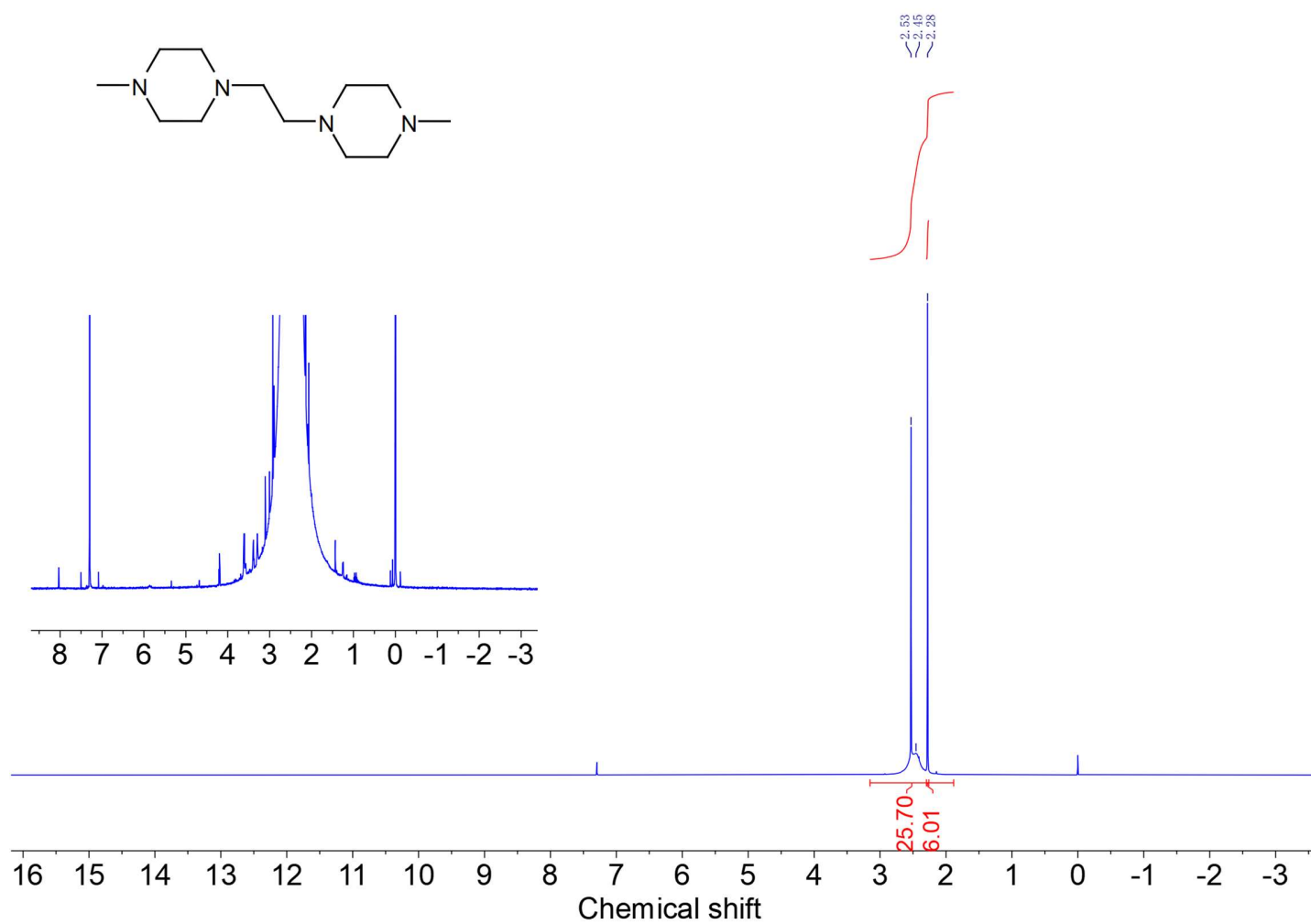


Figure S22. ¹H NMR spectrum of 1,2-bis(4-methylpiperazin-1-yl)ethane **10** (500 MHz, chloroform-d).

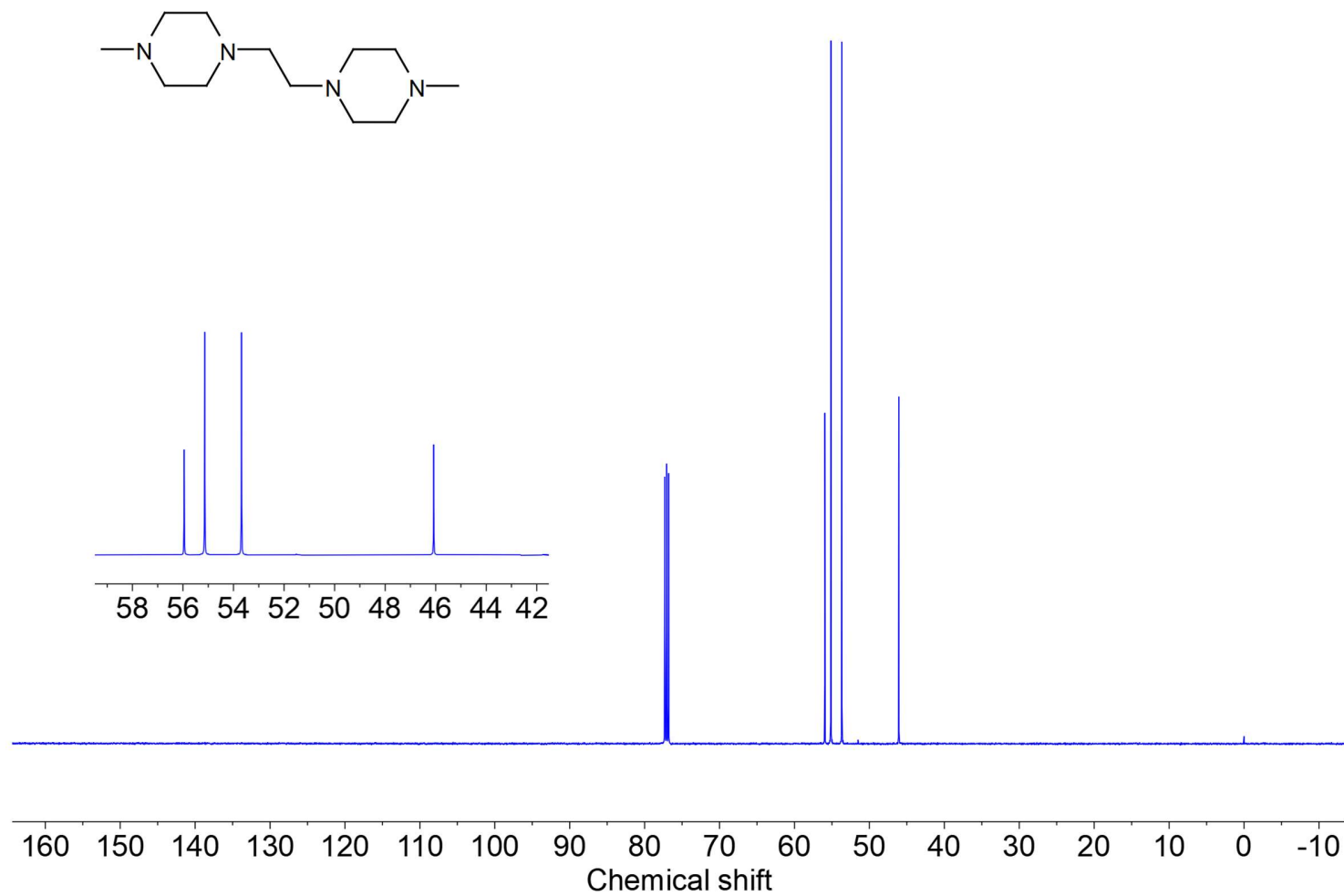


Figure S23. ^{13}C NMR spectrum of 1,2-bis(4-methylpiperazin-1-yl)ethane **10** (126 MHz, chloroform-d).

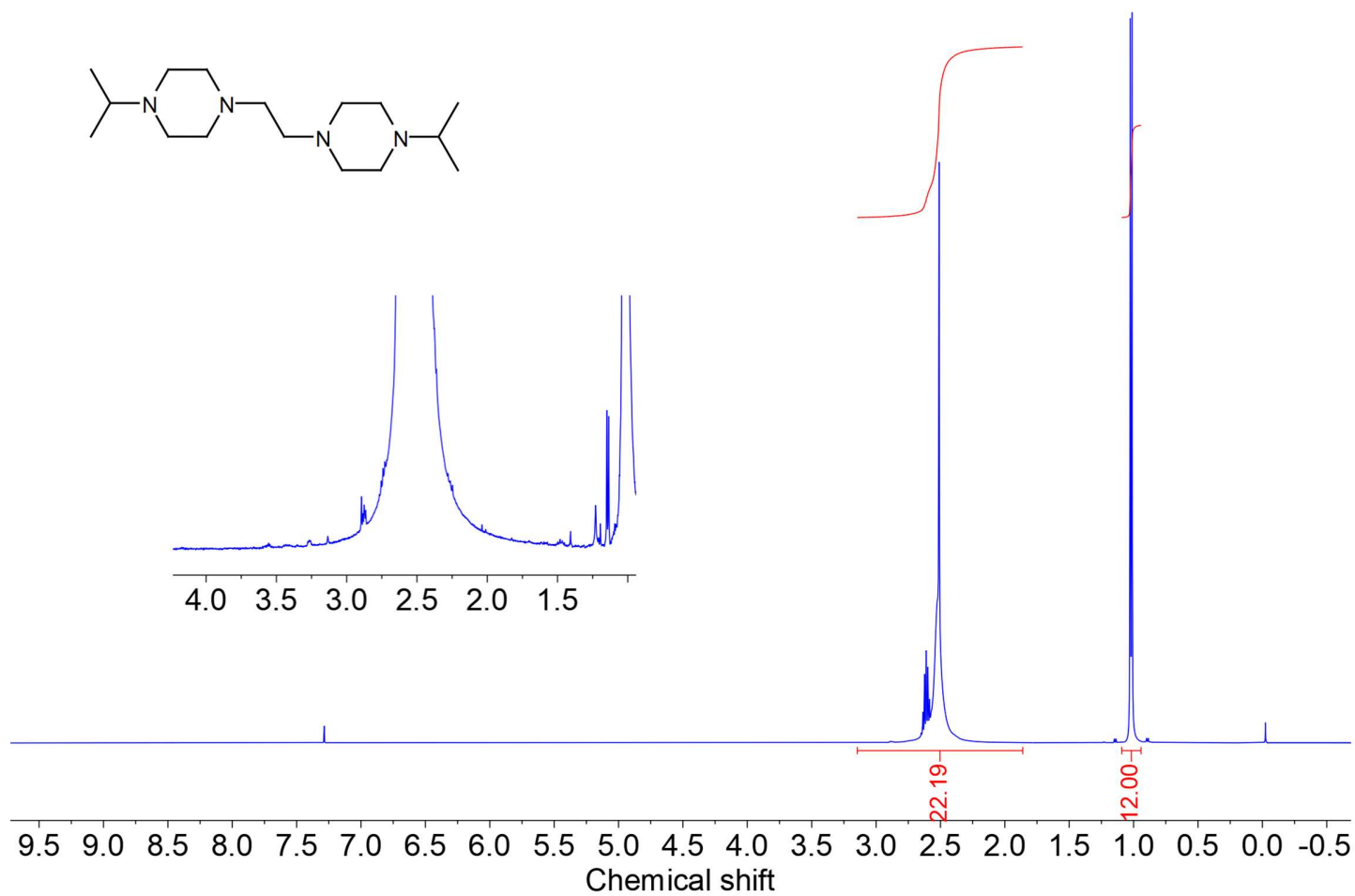


Figure S24. ^1H NMR spectrum of 1,2-bis(4-isopropylpiperazin-1-yl)ethane **11** (500 MHz, chloroform- d).

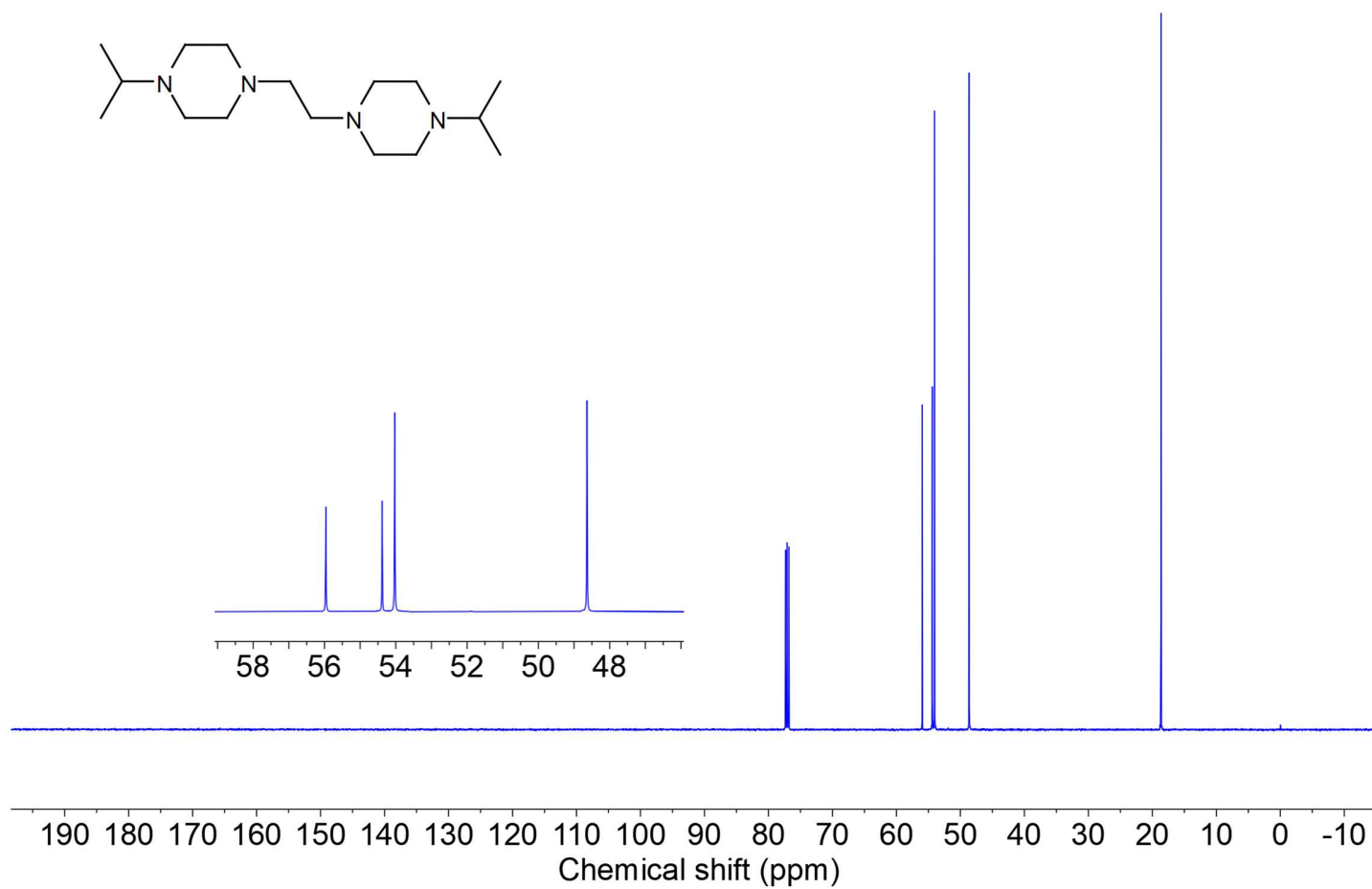


Figure S25. ^{13}C NMR spectrum of 1,2-bis(4-isopropylpiperazin-1-yl)ethane **11** (500 MHz, chloroform-d).

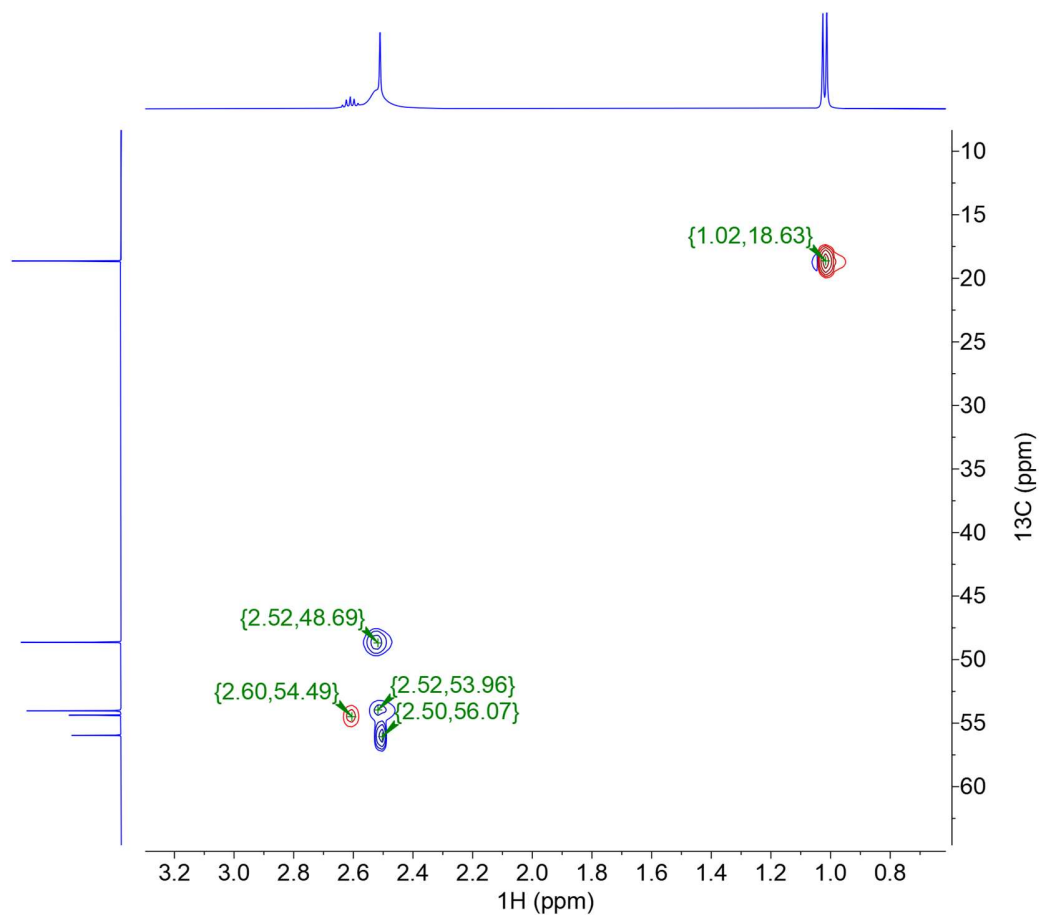


Figure S26. ^1H - ^{13}C HSQC spectrum of 1,2-bis(4-isopropylpiperazin-1-yl)ethane **11** (500 MHz, chloroform- d).

Spectroscopic Data — NMR Spectra of Allyltin and Allyllithium Complexes

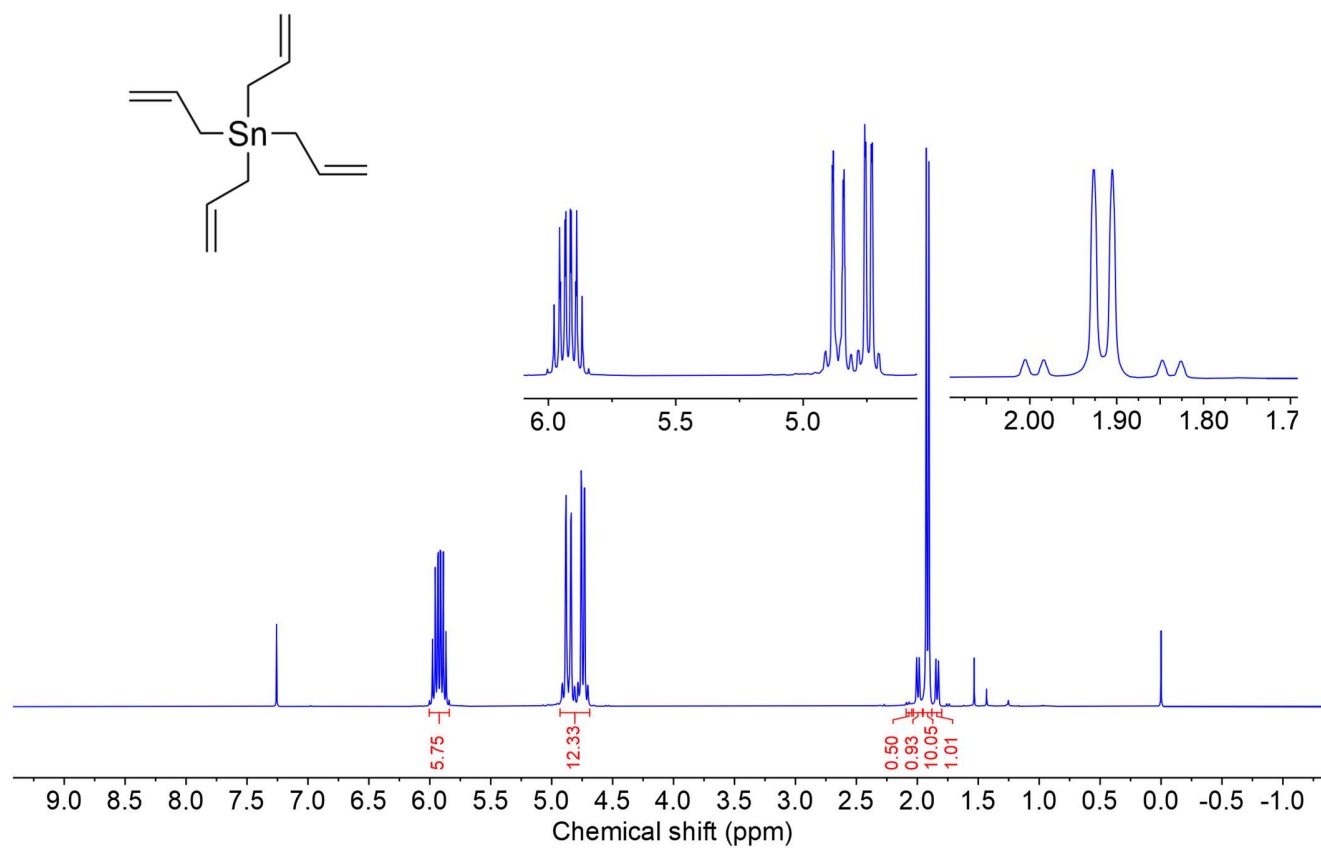


Figure S27. ^1H NMR spectrum of tetraallyltin (500 MHz, chloroform-d).

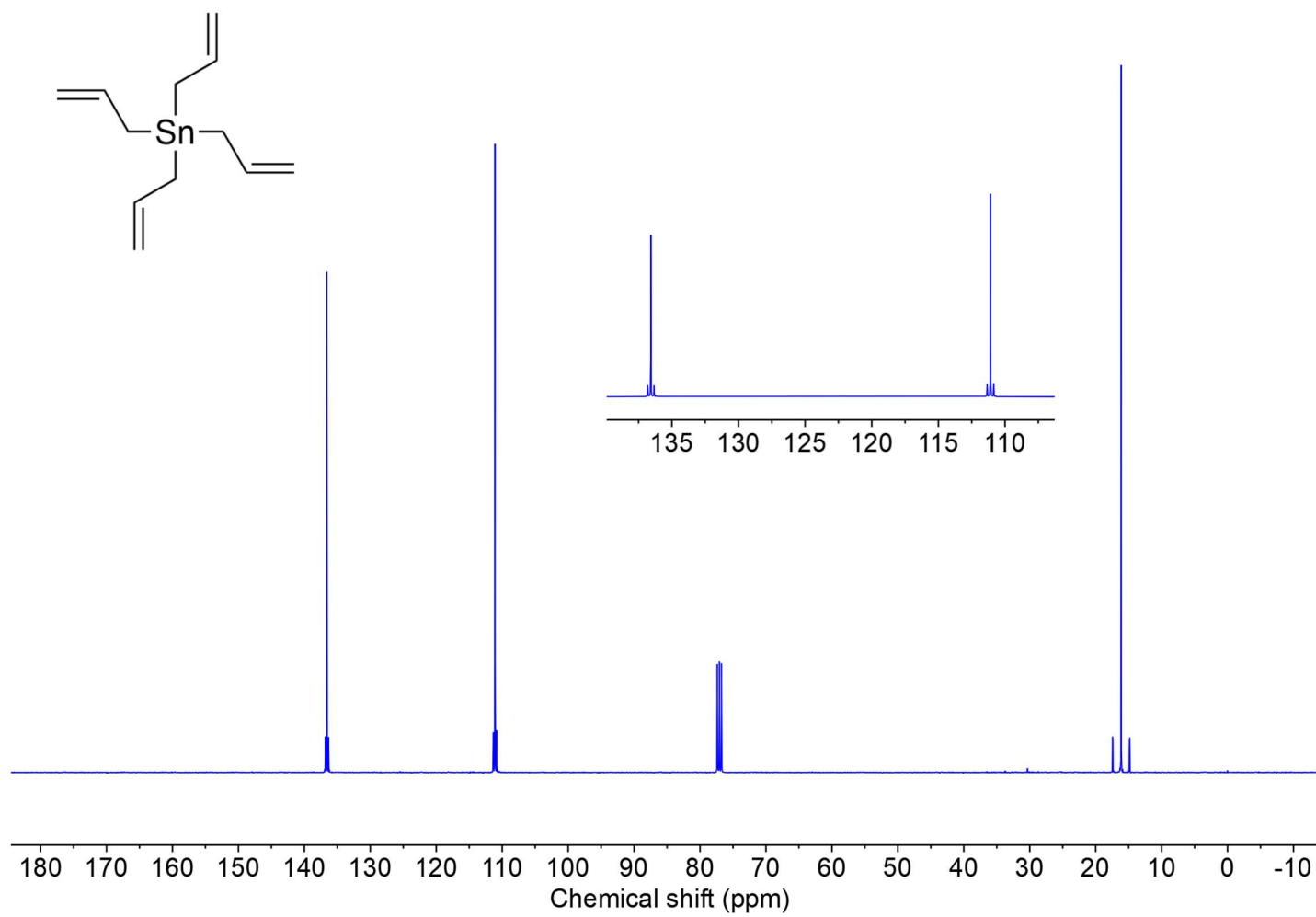


Figure S28. ^{13}C NMR spectrum of tetraallyltin (500 MHz, chloroform-d).

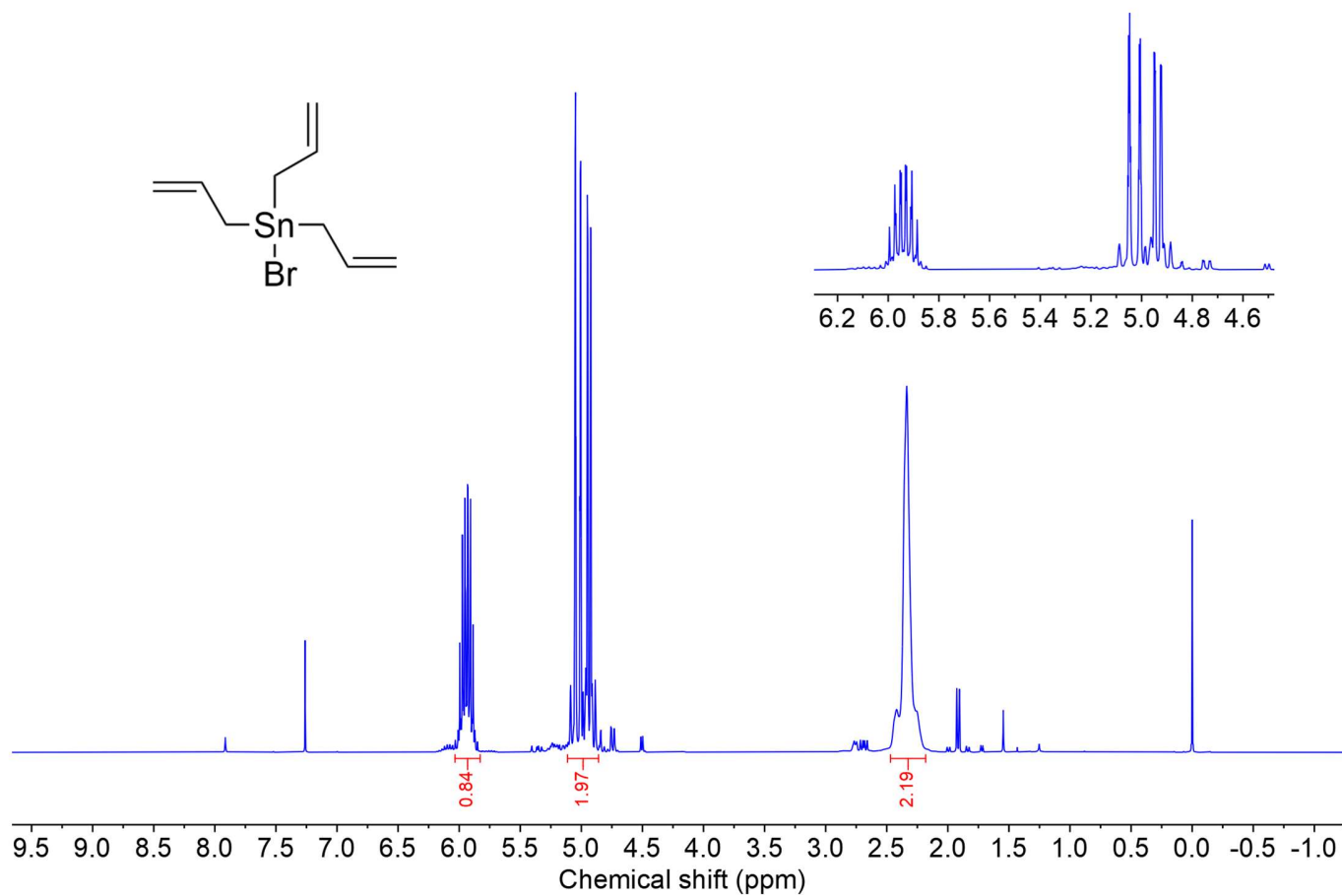


Figure S29. ^1H NMR spectrum of triallyltin bromide (500 MHz, chloroform-d).

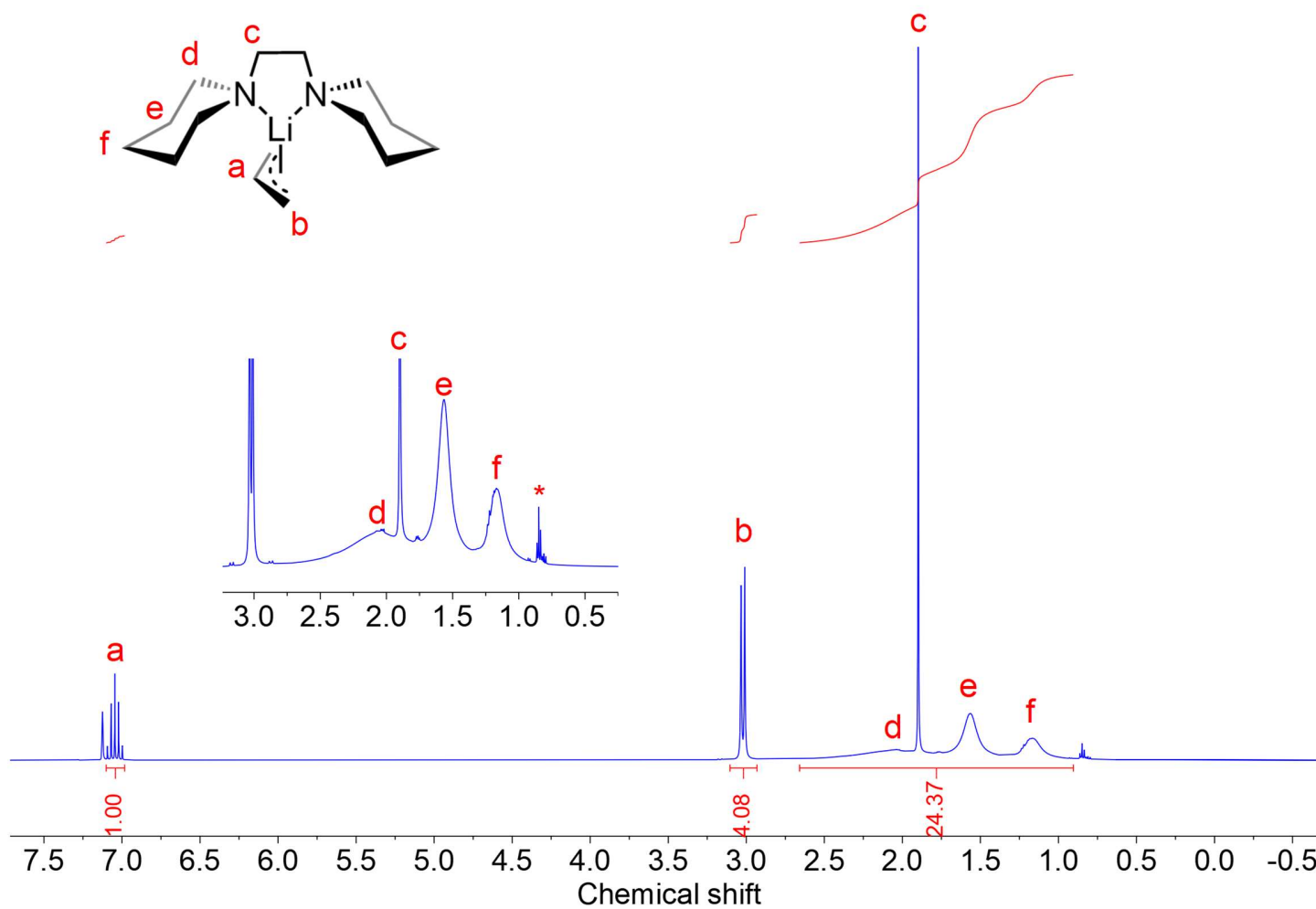


Figure S30. ^1H NMR spectrum of **6a** (500 MHz, benzene- d_6 , *aliphatic methyl proton signals of impurities).

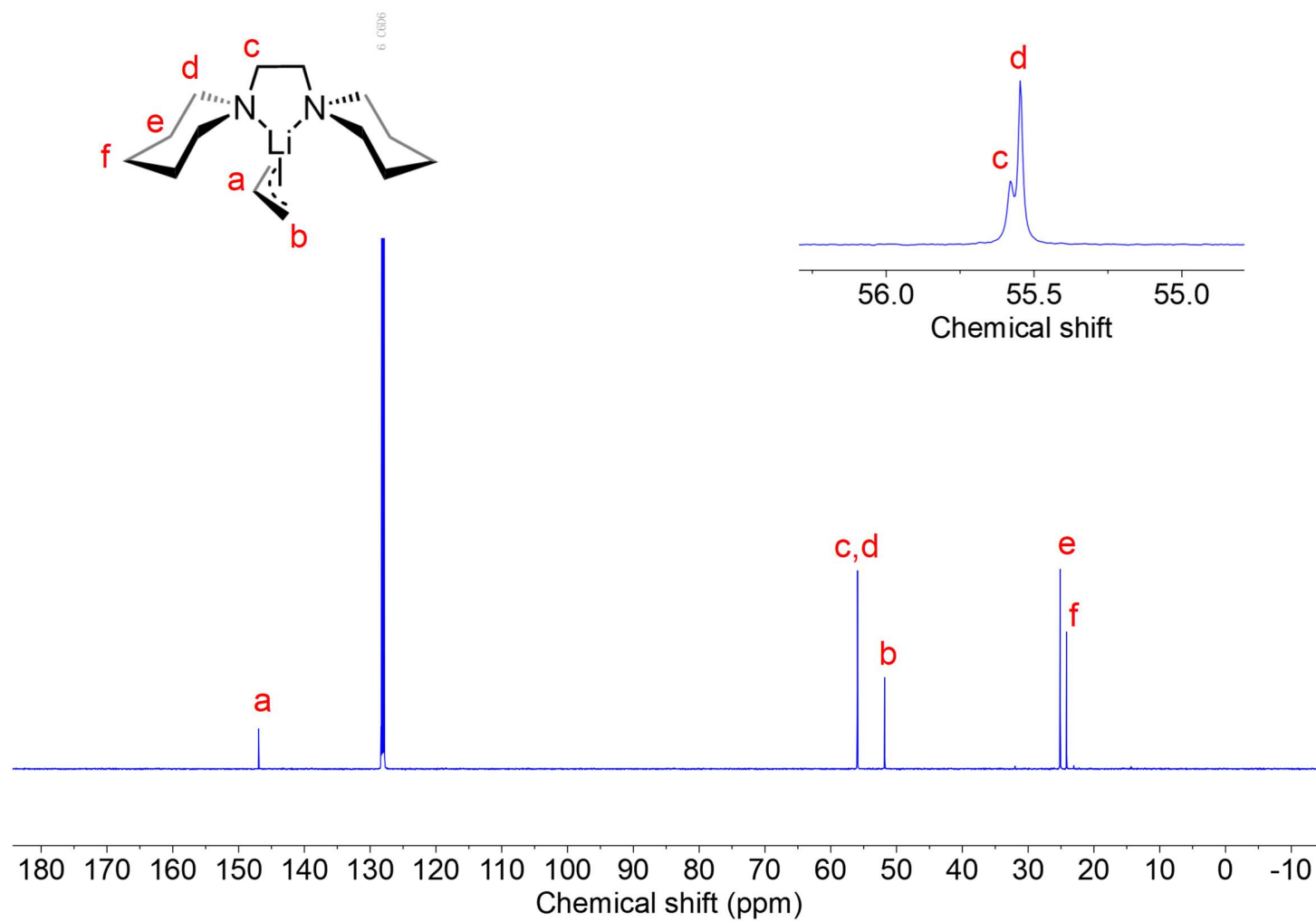


Figure S31. ^{13}C NMR spectrum of **6a** (126 MHz, benzene- d_6).

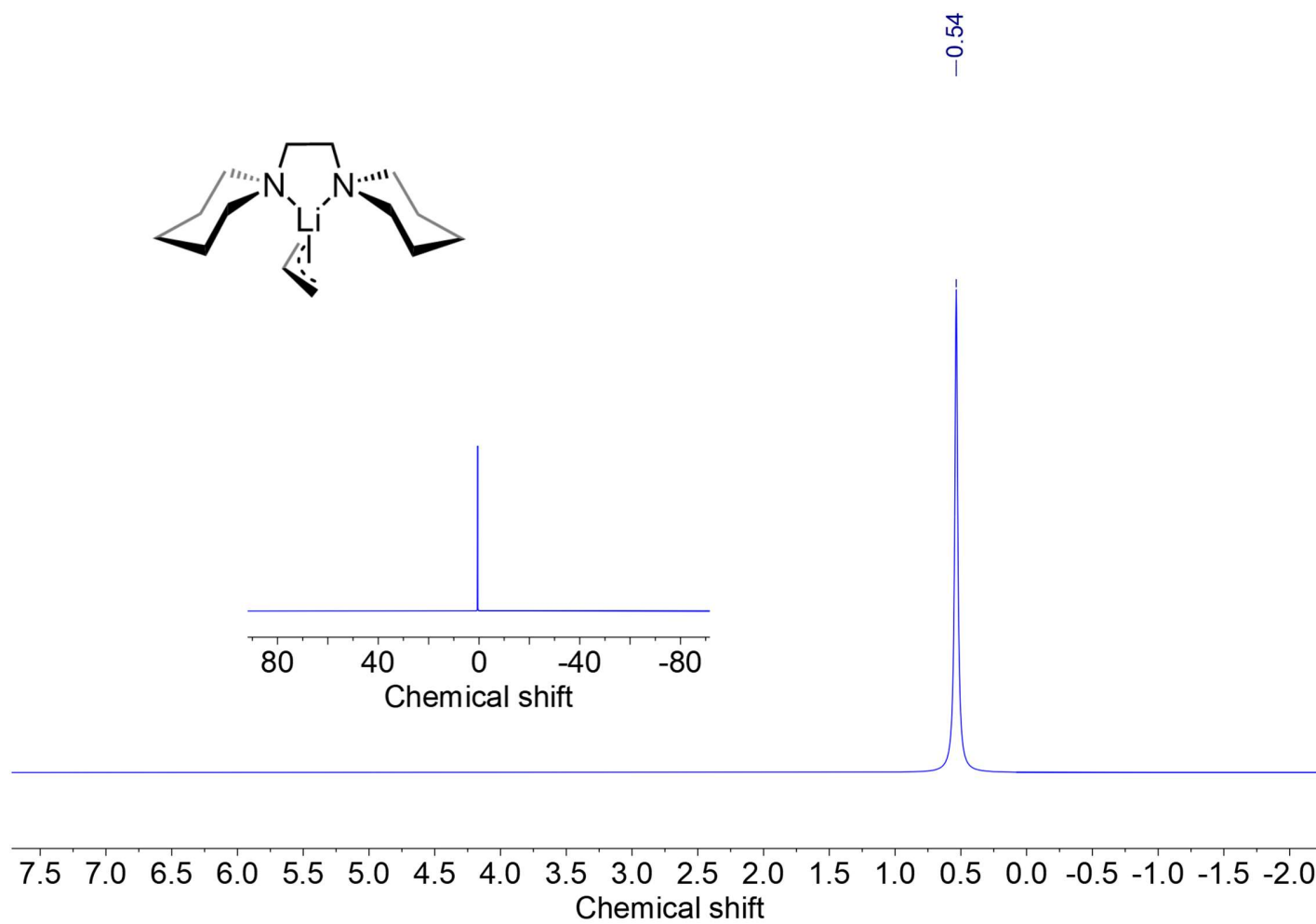


Figure S32. ^7Li NMR spectrum of **6a** (126 MHz, benzene- d_6).

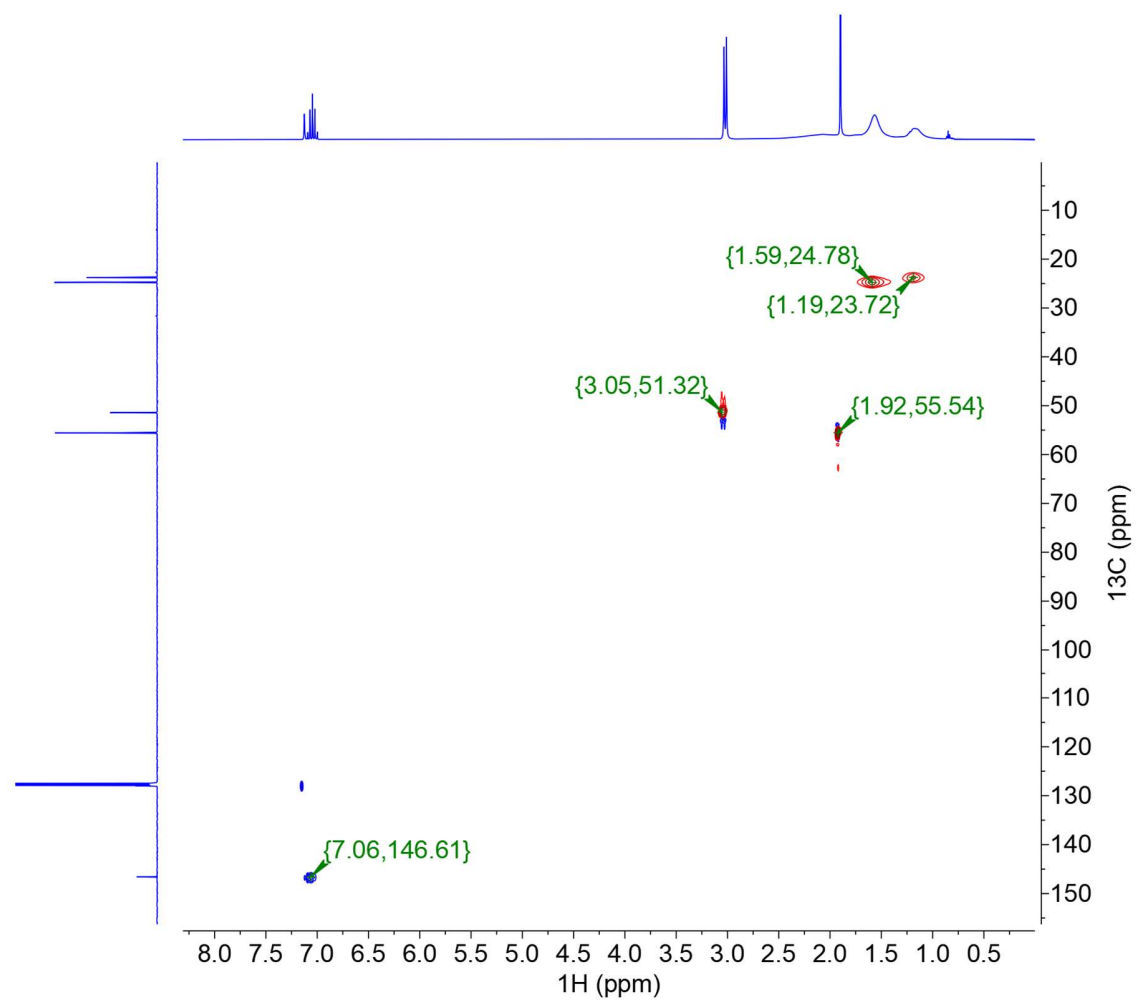


Figure S33. ^1H - ^{13}C HSQC NMR spectrum of **6a** (500/100 MHz, benzene- d_6).

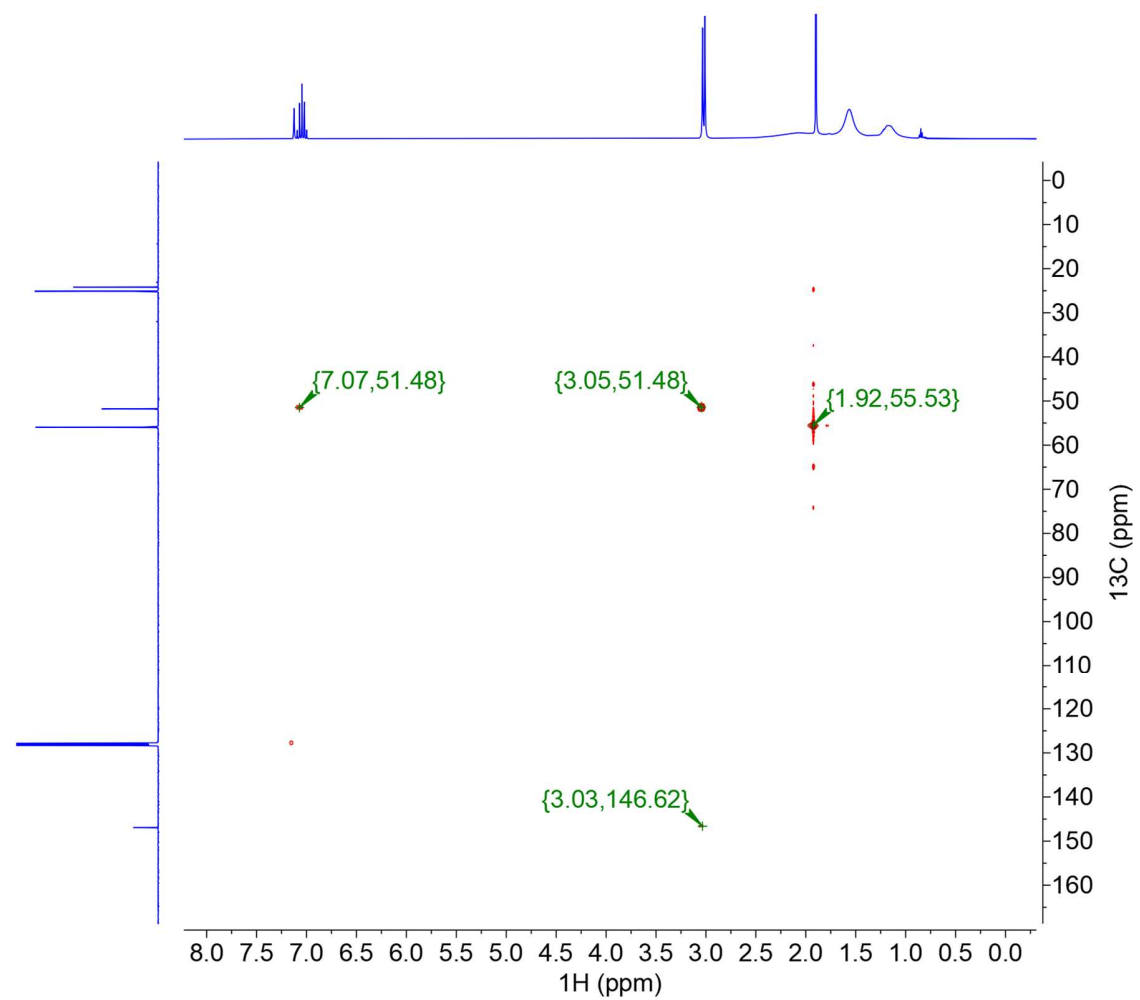


Figure S34. ^1H - ^{13}C HMBC NMR spectrum of **6a** (194 MHz, benzene- d_6).

Spectroscopic Data — ^{13}C NMR Spectra of “Living” Polybutadiene with Lewis Bases

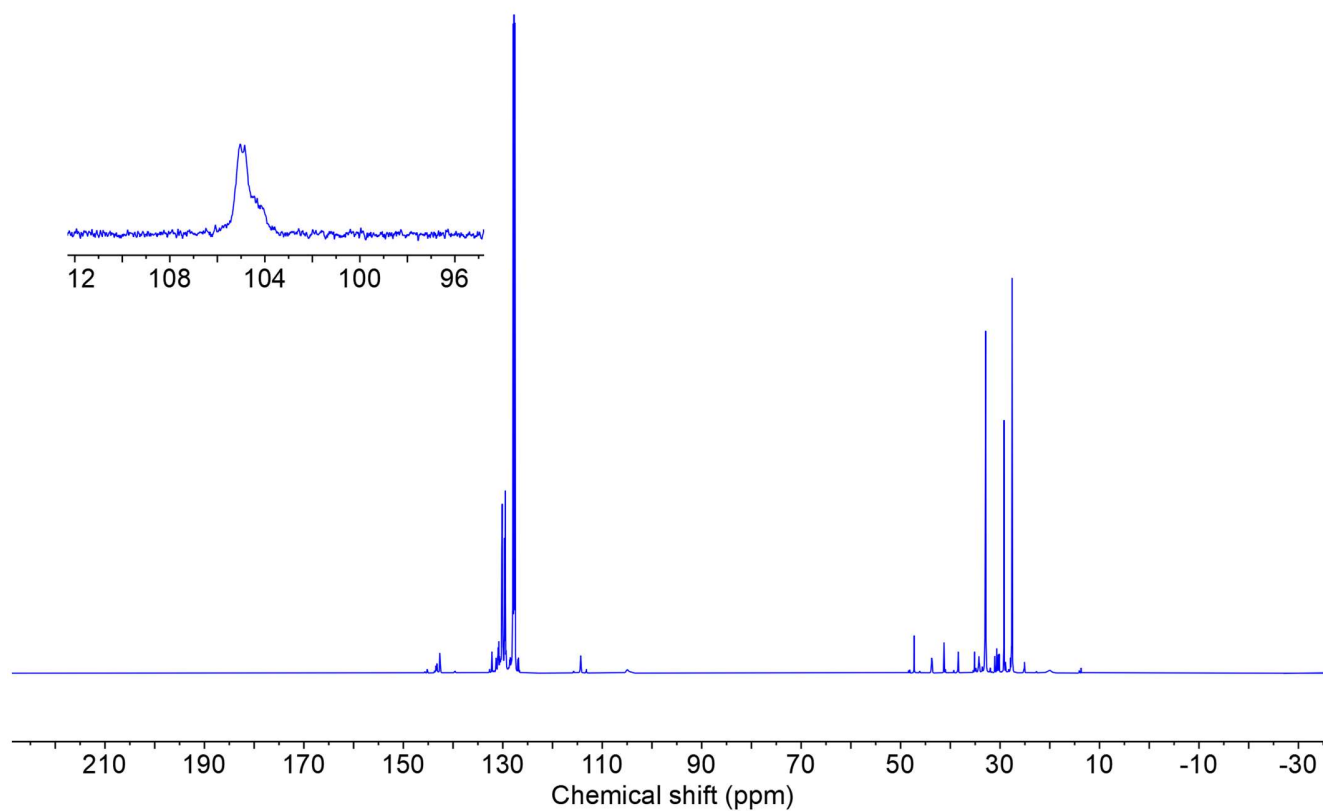


Figure S35. ^{13}C NMR spectrum of “living” polybutadiene (500 MHz, benzene- d_6).

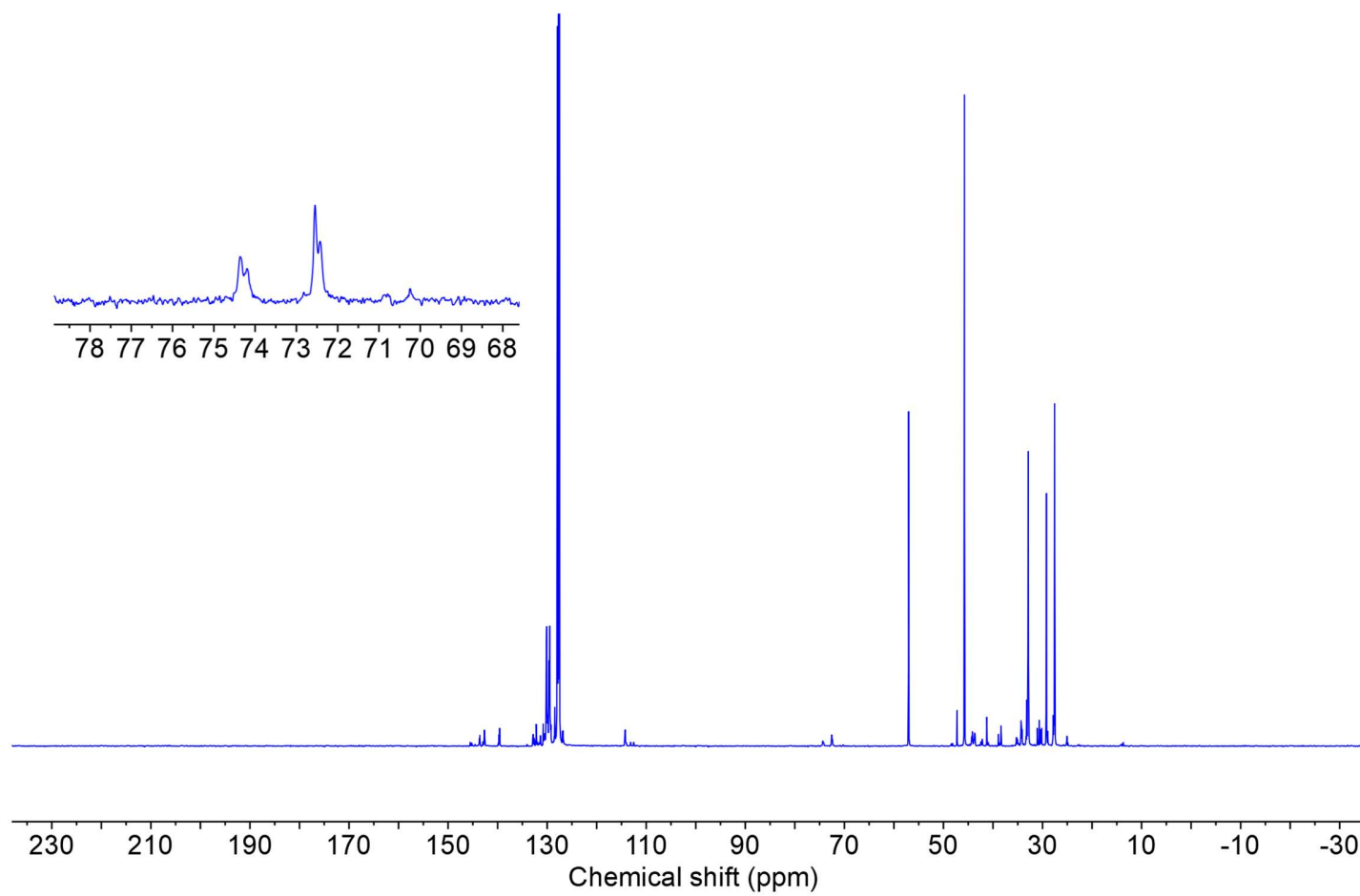


Figure S36. Effect of **3** TMEDA on ^{13}C NMR spectrum of "living" polybutadiene (500 MHz, benzene- d_6).

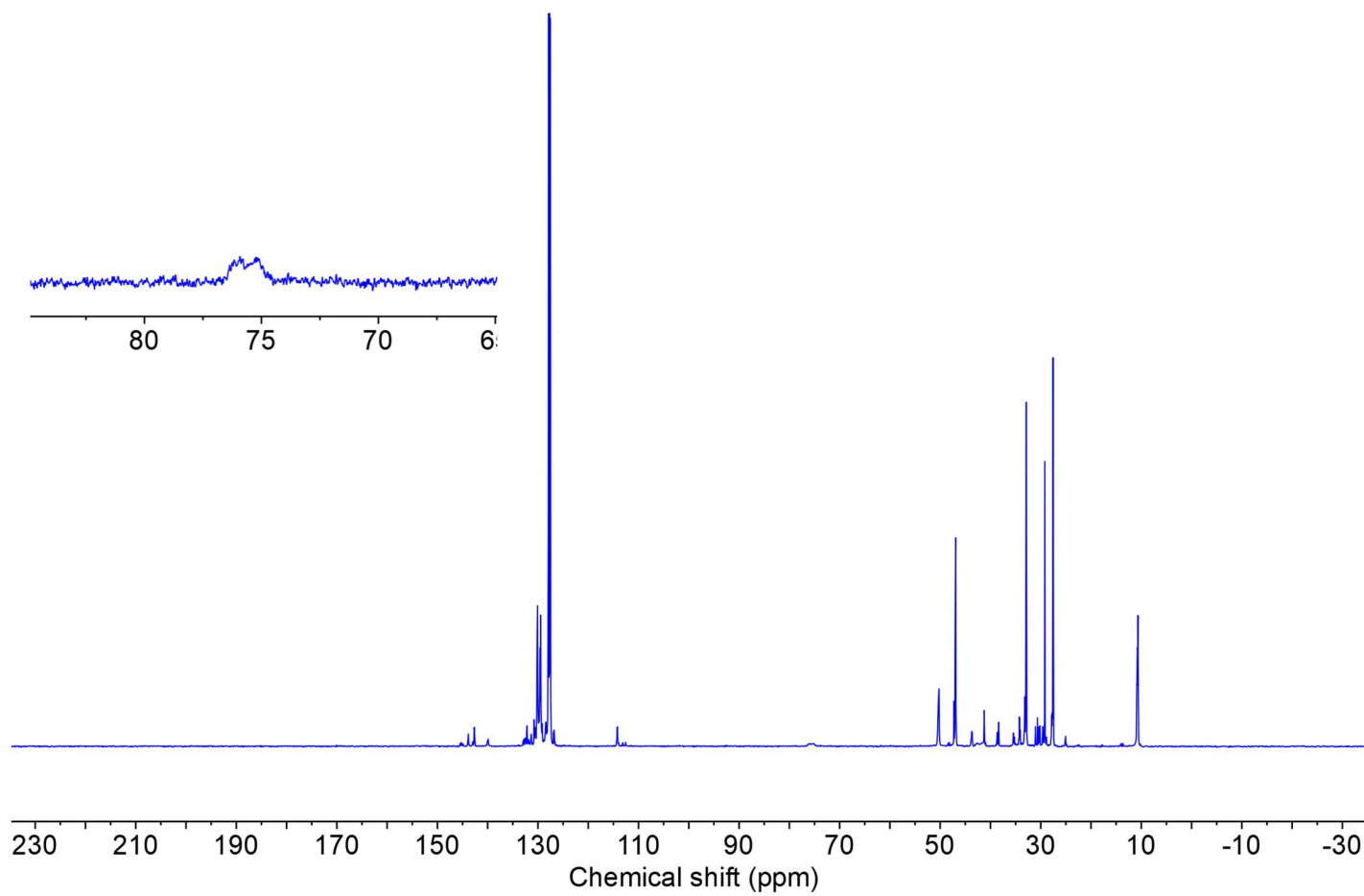


Figure S37. Effect of **4** TEEDA on ^{13}C NMR spectrum of "living" polybutadiene (500 MHz, benzene- d_6).

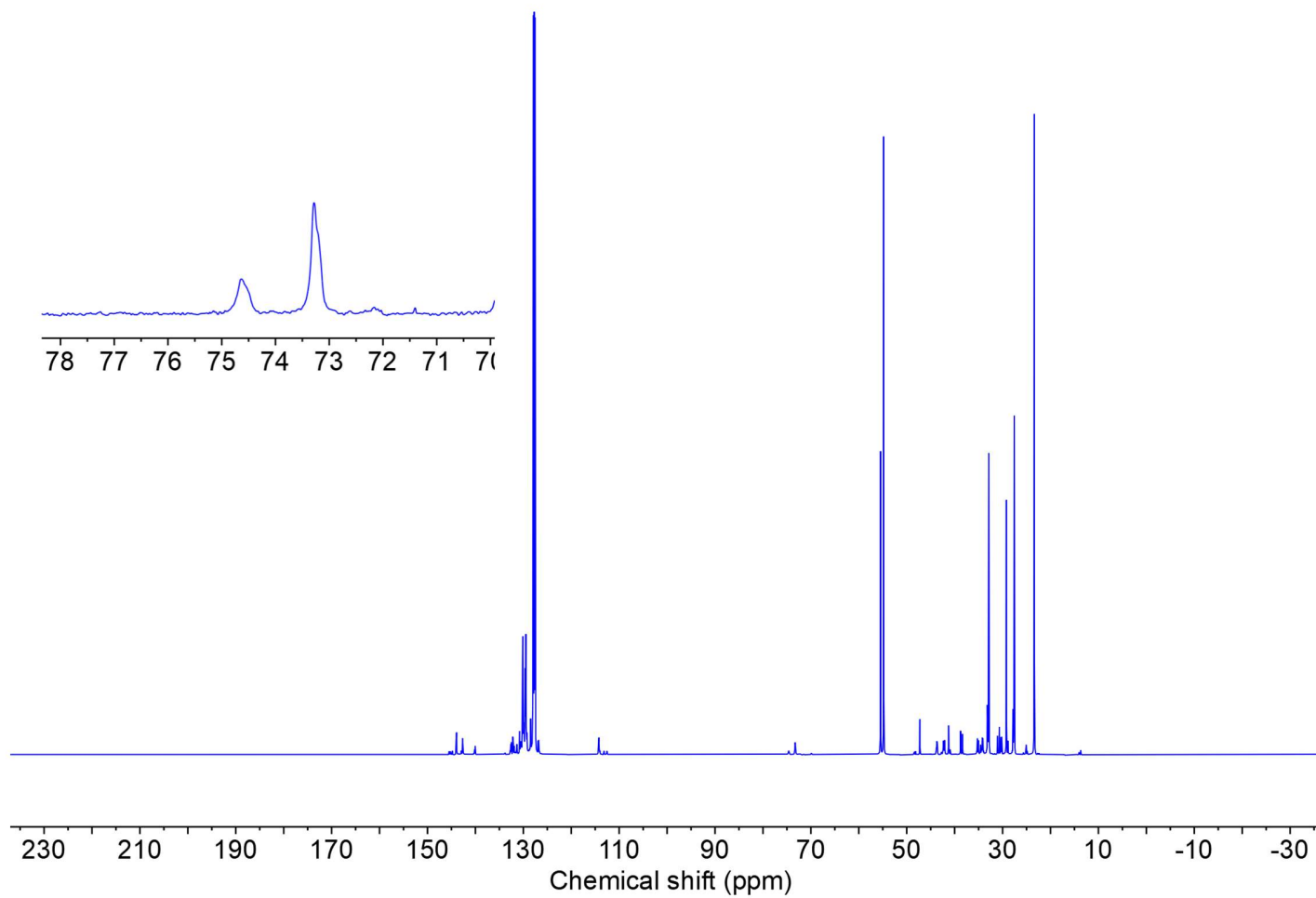


Figure S38. Effect of **5** DiPyr on ^{13}C NMR spectrum of "living" polybutadiene (500 MHz, benzene- d_6).

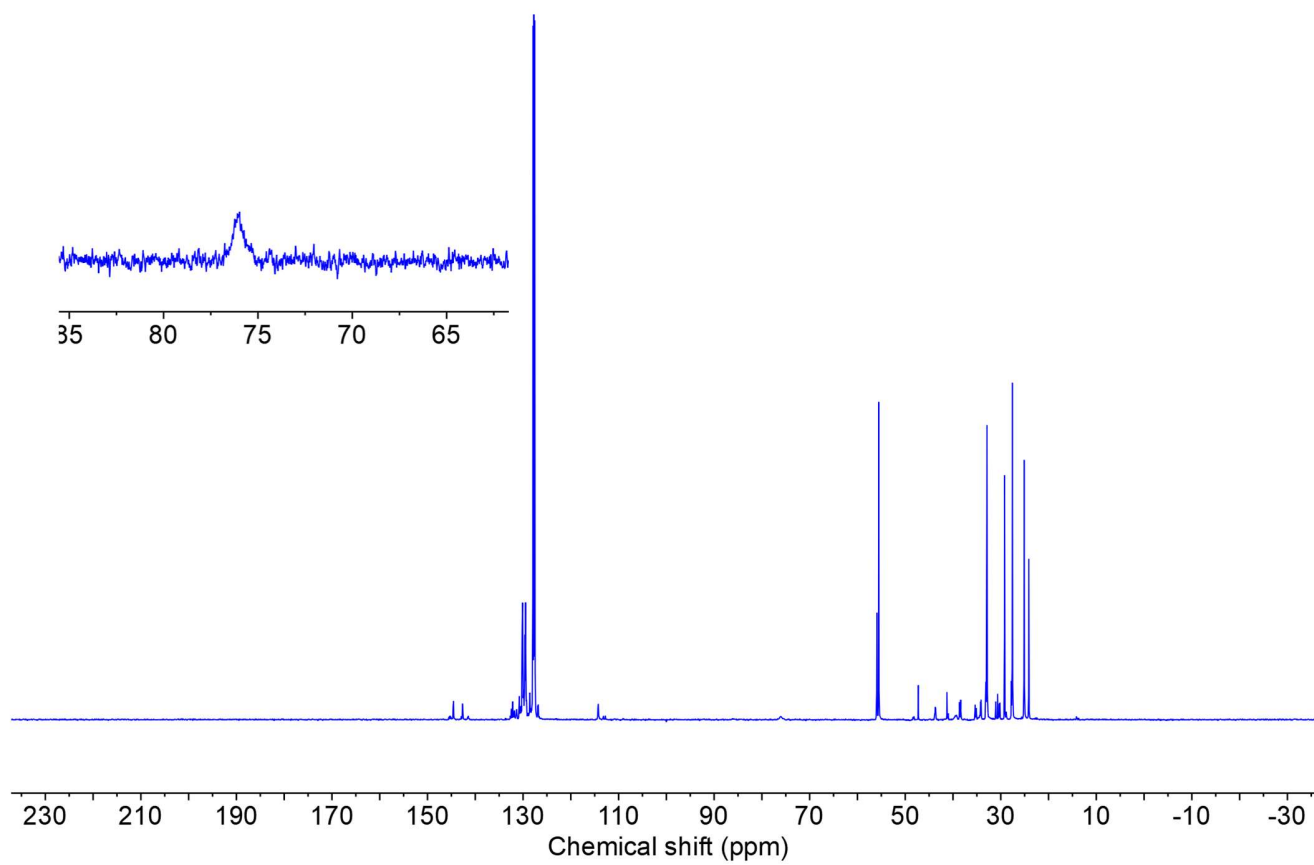


Figure S39. Effect of 6 DiPip on ^{13}C NMR spectrum of "living" polybutadiene (500 MHz, benzene- d_6).

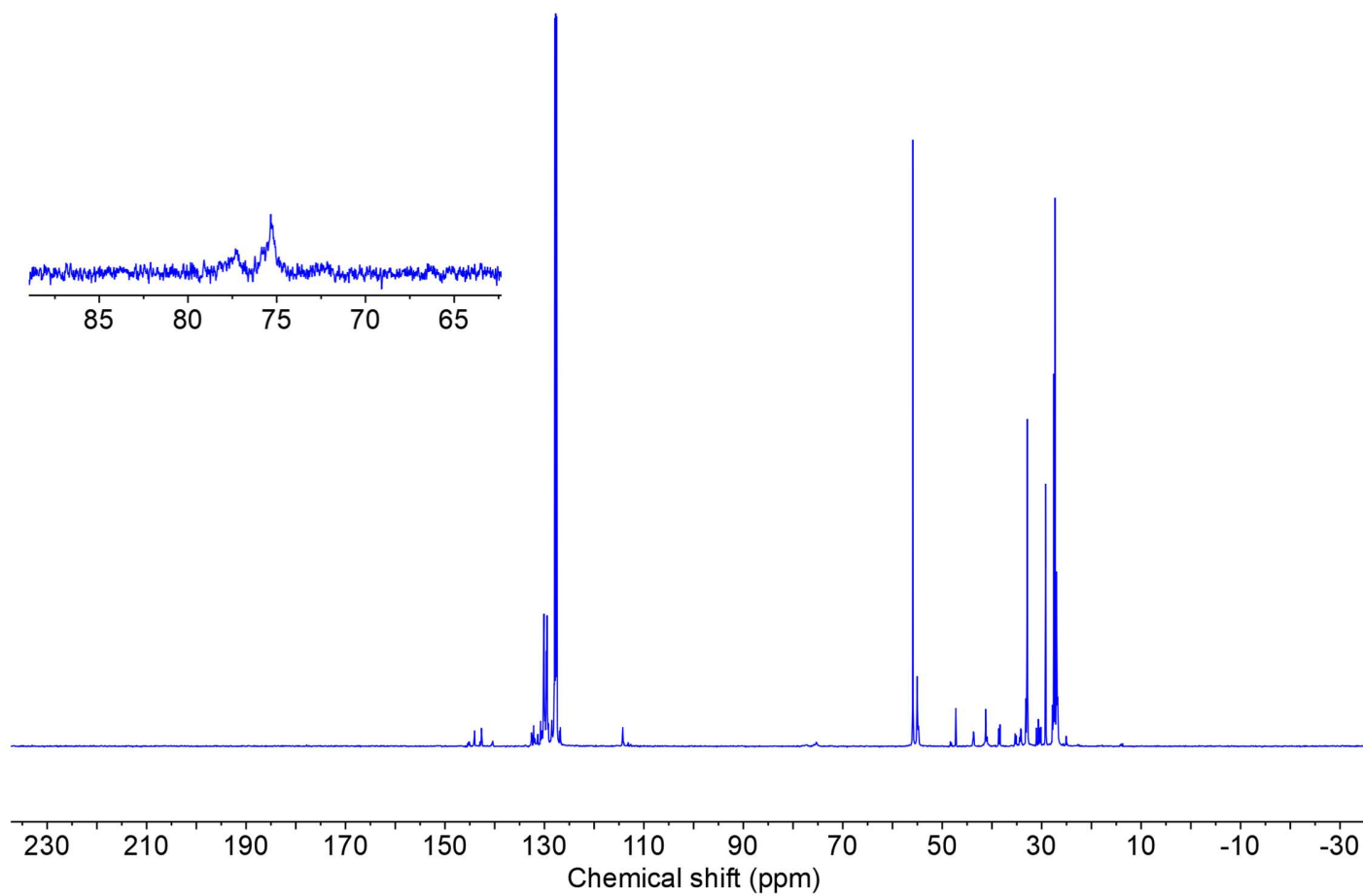


Figure S40. Effect of **7** DiAze on ^{13}C NMR spectrum of "living" polybutadiene (500 MHz, benzene- d_6).

Spectroscopic Data — ^1H NMR Spectra of Selectively Deuterated Polybutadienyllithium with Lewis Bases

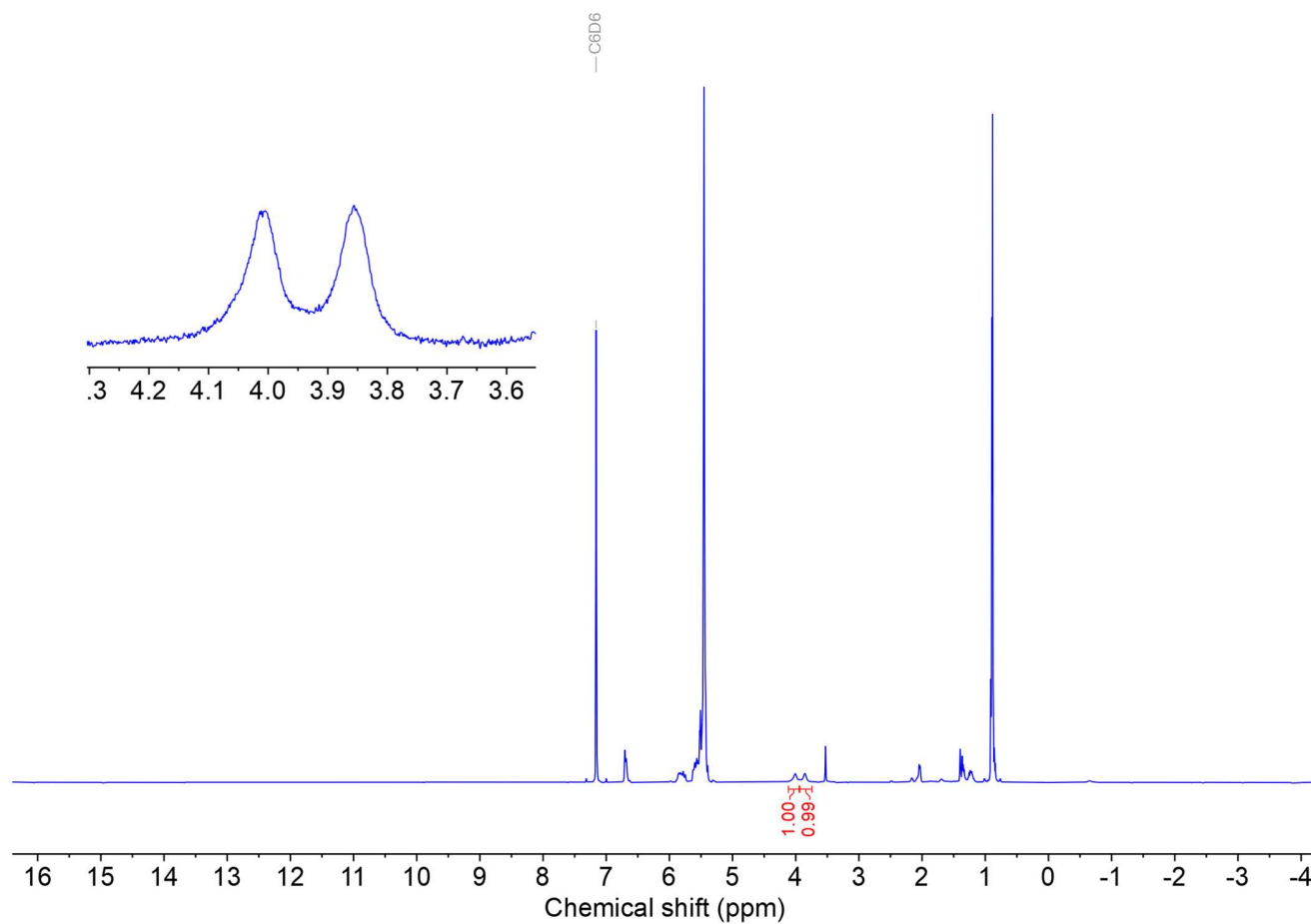


Figure S41. ^1H NMR spectrum of selectively deuterated polybutadienyllithium/THF- d_8 (500 MHz, benzene- d_6).

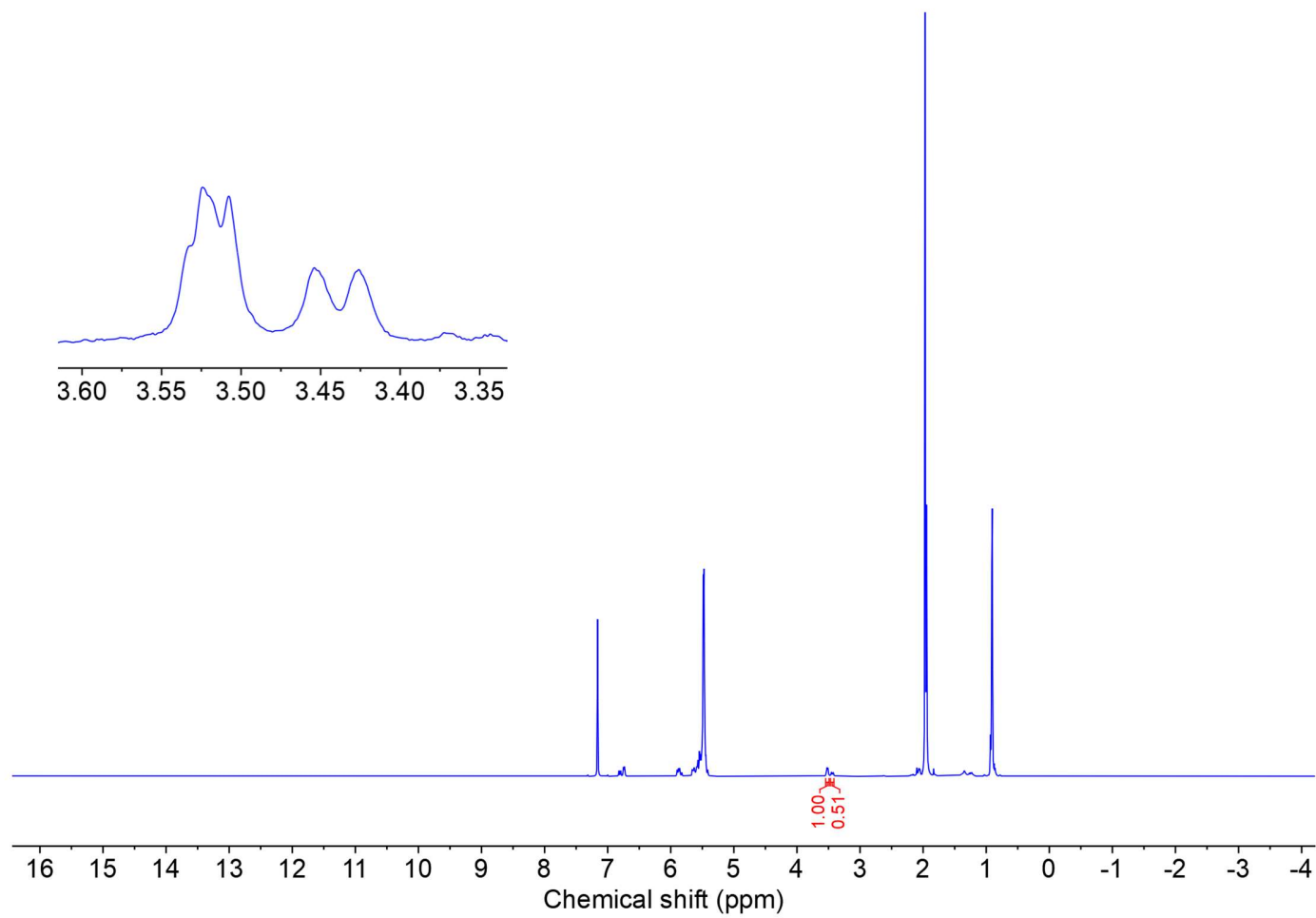


Figure S42. ^1H NMR spectrum of selectively deuterated polybutadienyllithium/**3** TMEDA (500 MHz, benzene- d_6).

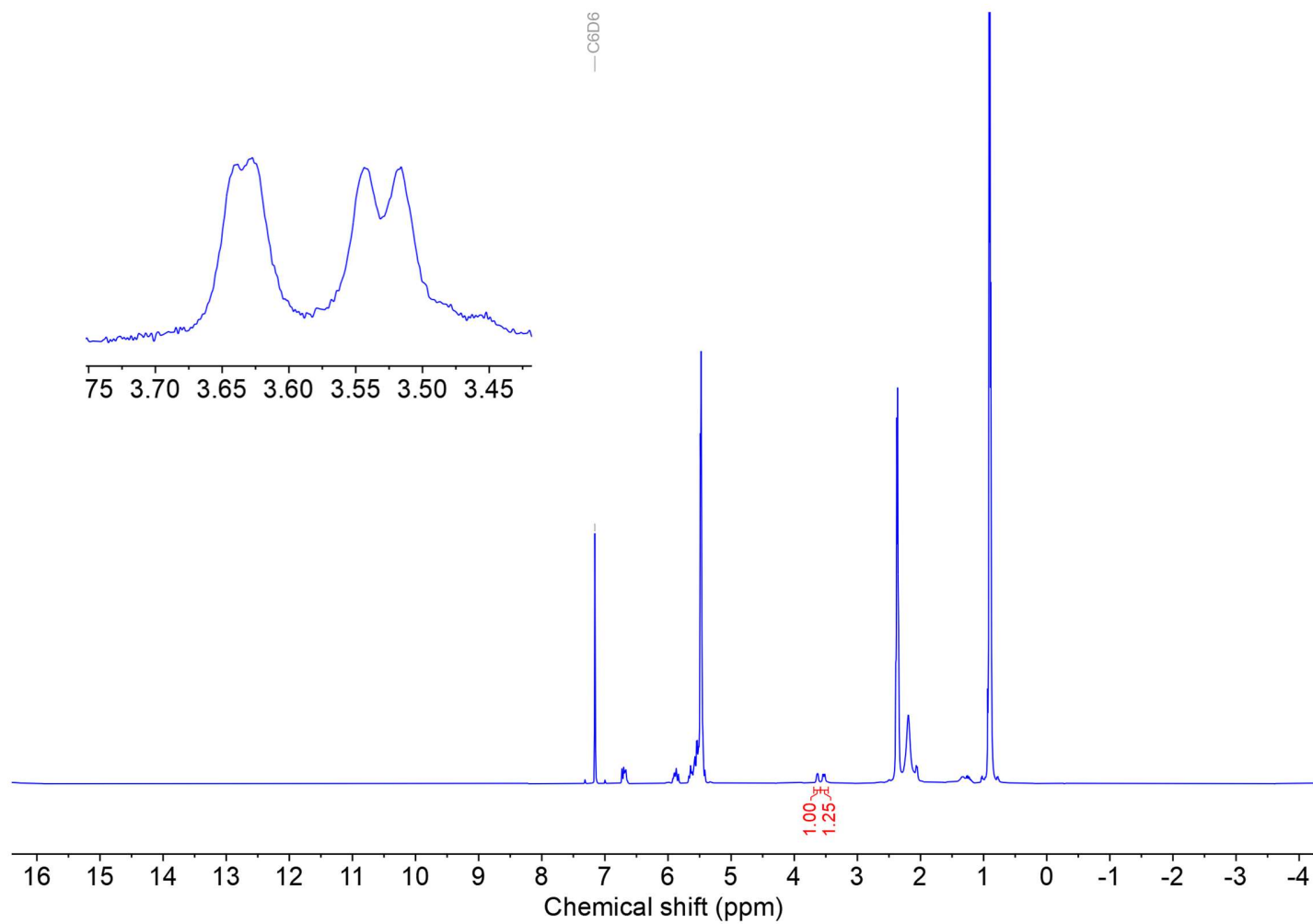


Figure S43. ^1H NMR spectrum of selectively deuterated polybutadienyllithium/4 TEEDA (500 MHz, benzene- d_6).

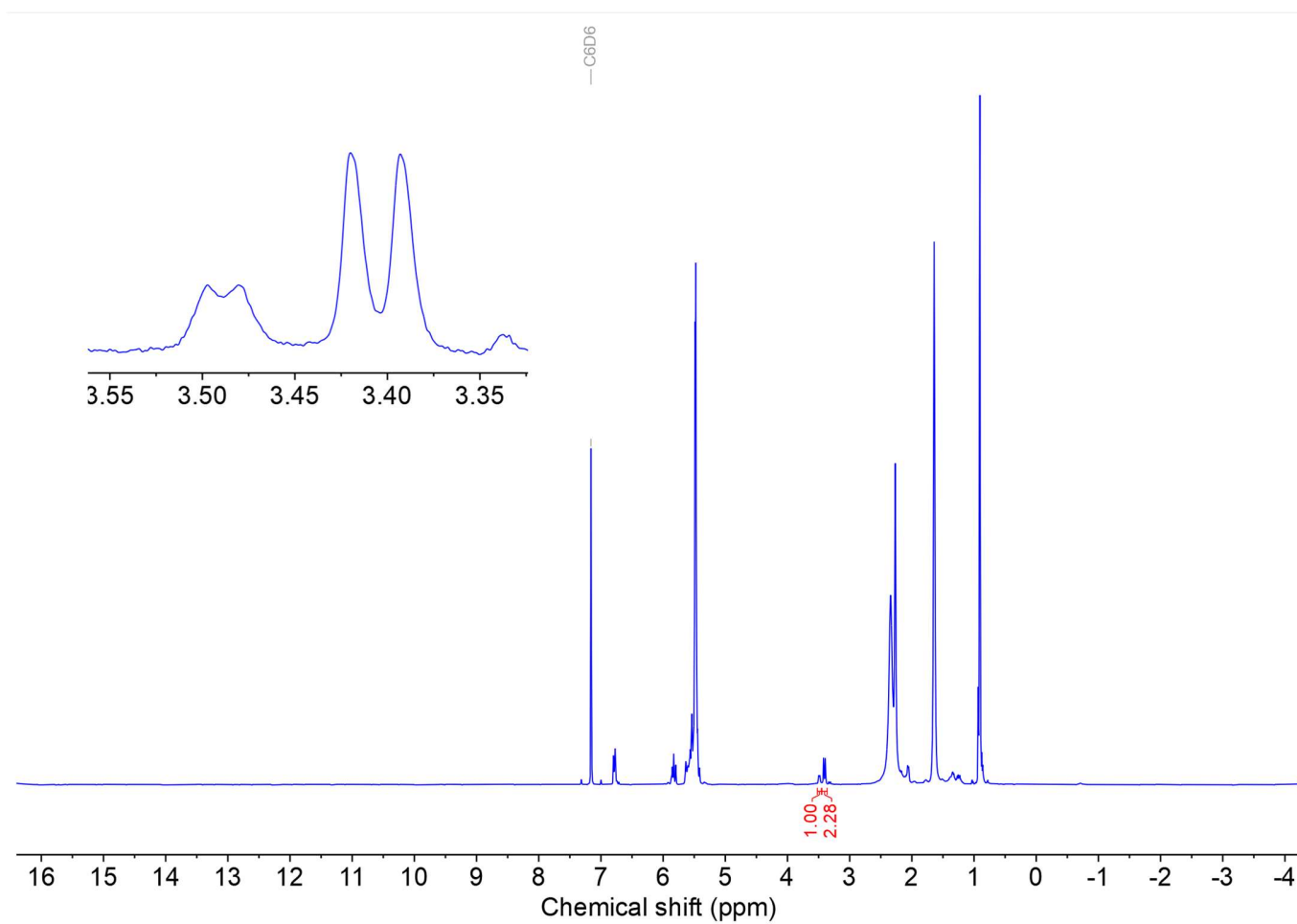


Figure S44. ^1H NMR spectrum of selectively deuterated polybutadienyllithium/5 DiPyr (500 MHz, benzene- d_6).

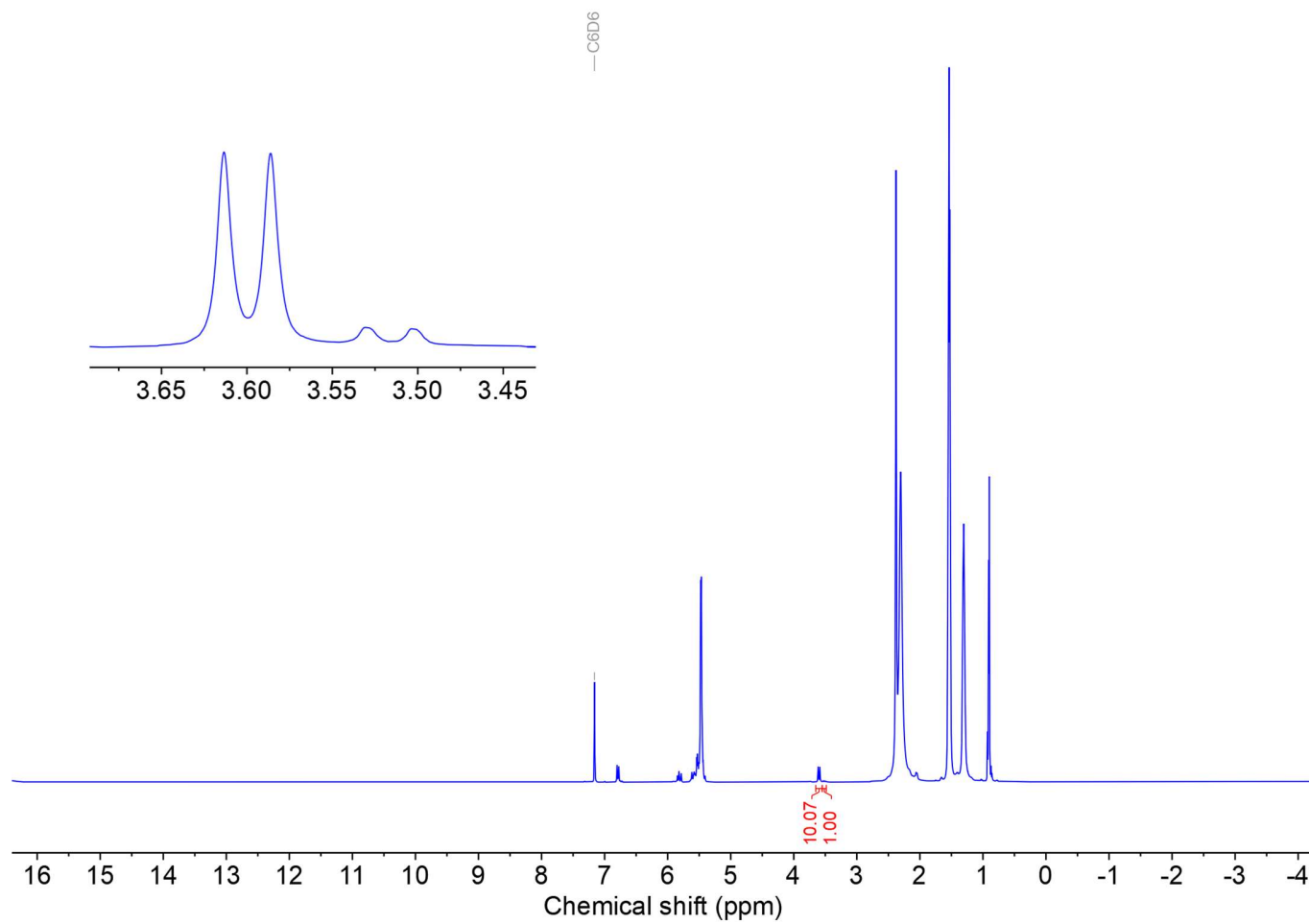


Figure S45. ^1H NMR spectrum of selectively deuterated polybutadienyllithium/6 DiPip (500 MHz, benzene- d_6).

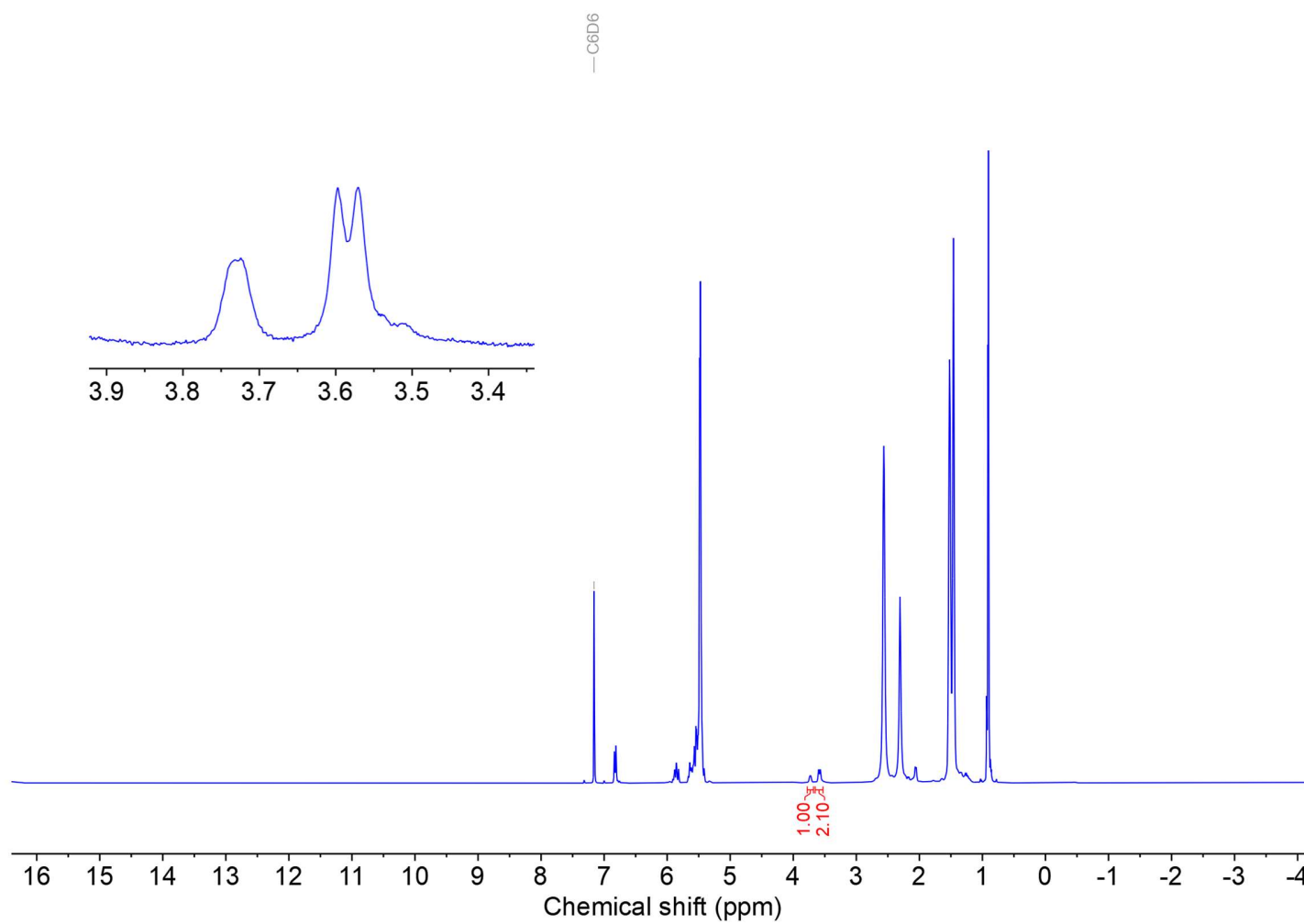


Figure S46. ^1H NMR spectrum of selectively deuterated polybutadienyllithium/7 DiAze (500 MHz, benzene- d_6).

Spectroscopic Data — ^2H NMR Spectra of Lewis Bases/*n*-BuLi Initiated Polybutadiene Terminated by MeOD

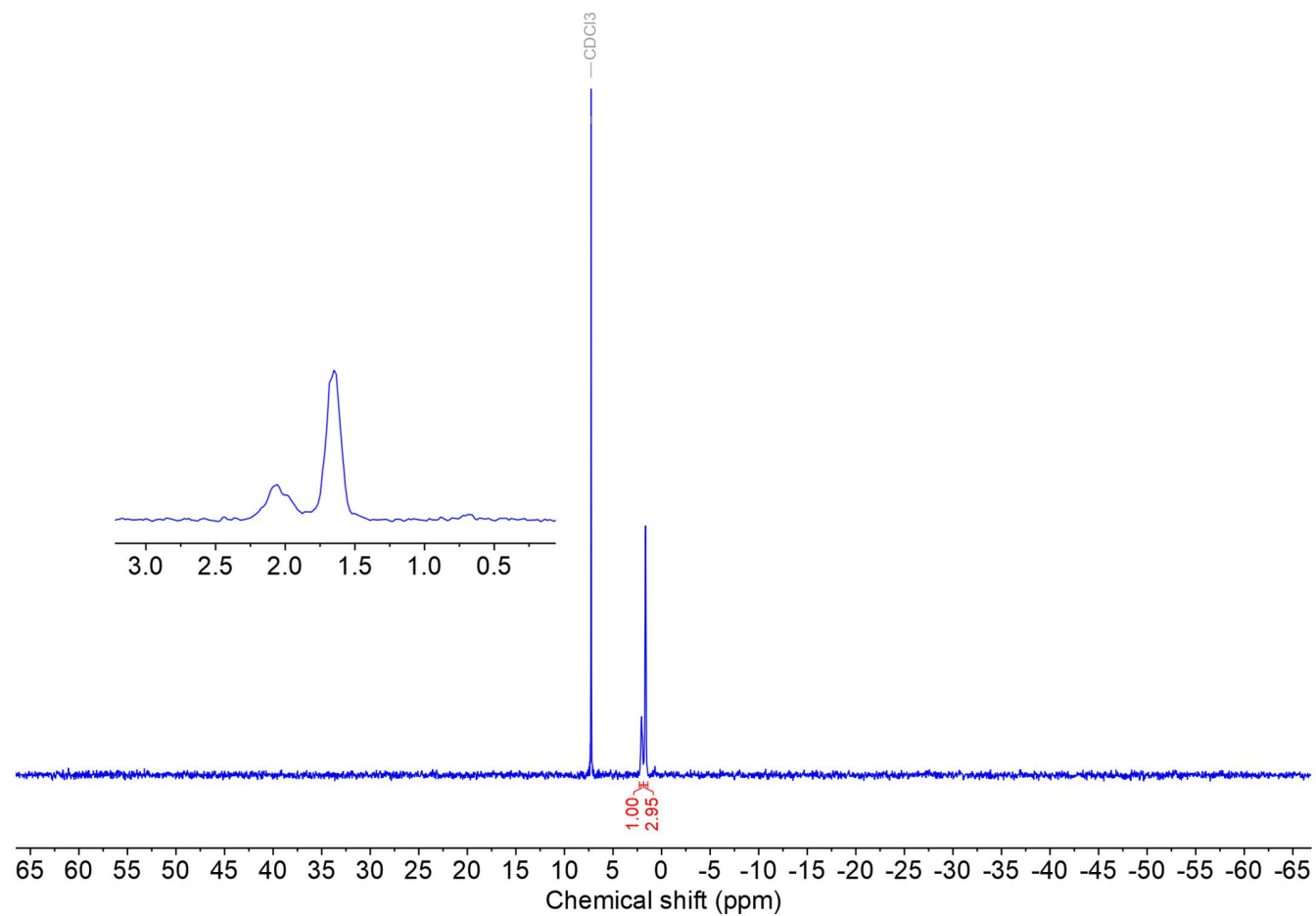


Figure S47. ^2H NMR spectrum of **1** glyme/*n*-BuLi initiated polybutadiene terminated by MeOD (61 MHz, chloroform-*d*).

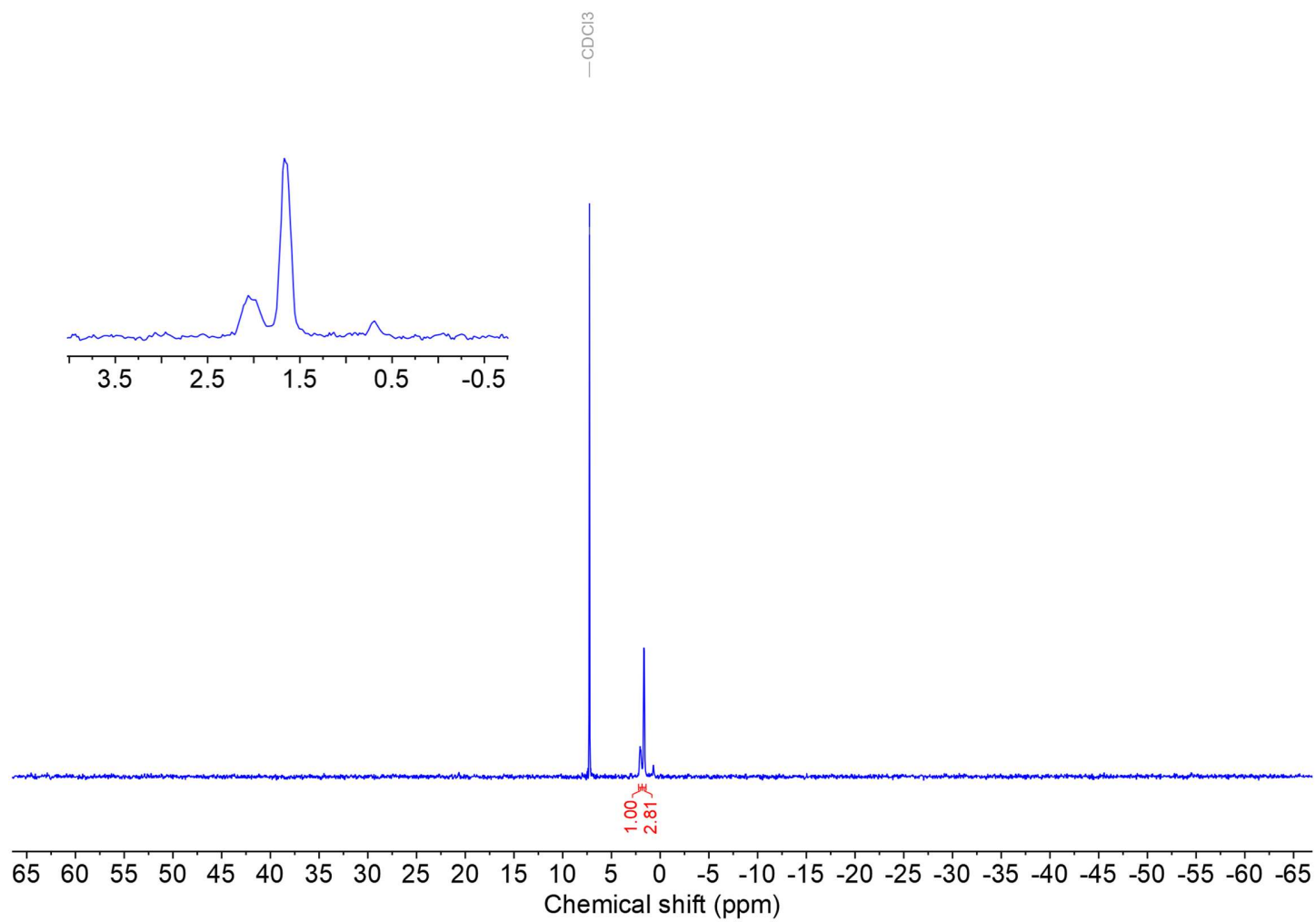


Figure S48. ^2H NMR spectrum of **2** THF/*n*-BuLi initiated polybutadiene terminated by MeOD (61 MHz, chloroform-*d*).

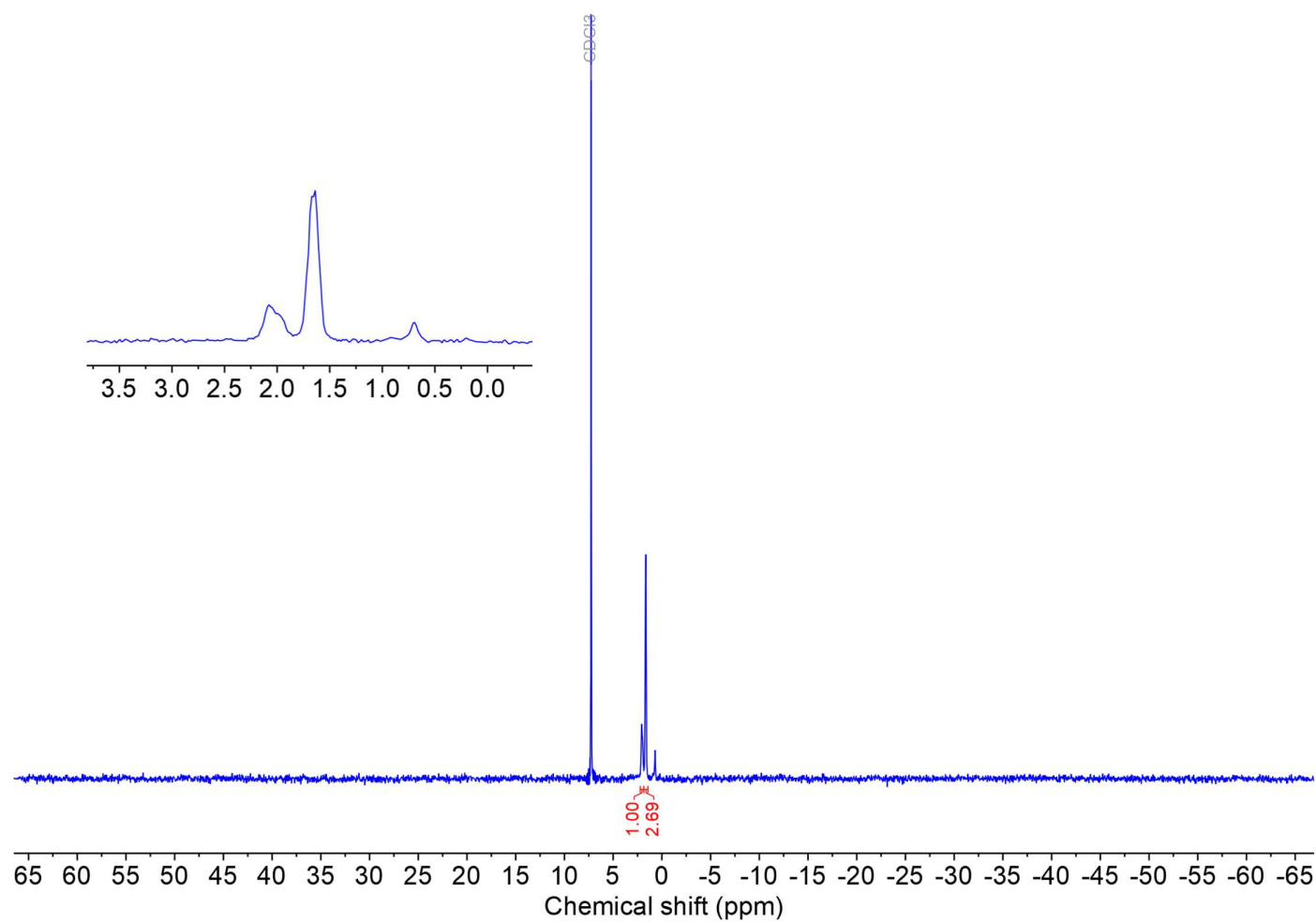


Figure S49. ^2H NMR spectrum of **3** TMEDA/*n*-BuLi initiated polybutadiene terminated by MeOD (61 MHz, chloroform-*d*).

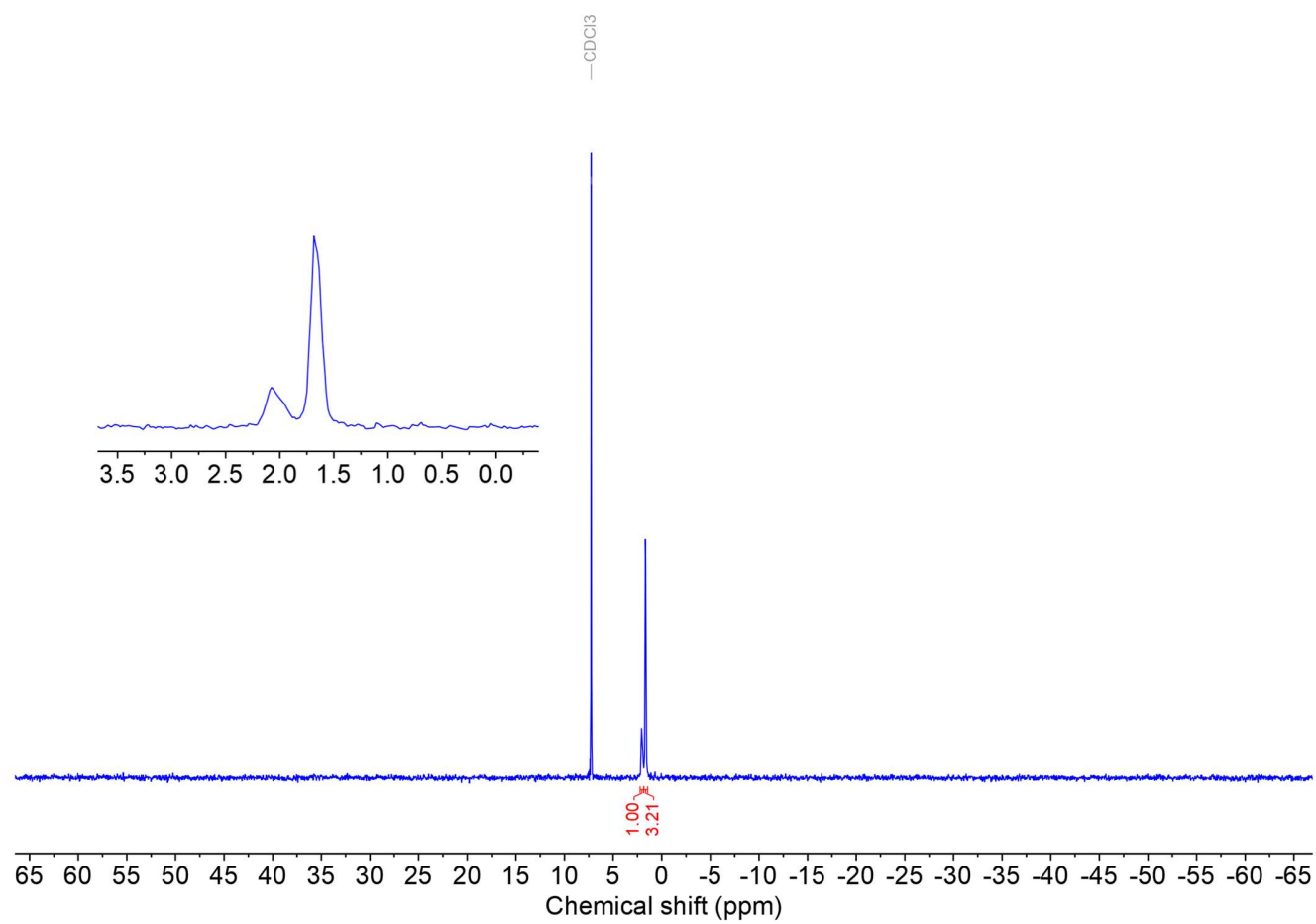


Figure S50. ^2H NMR spectrum of **4** TEEDA/*n*-BuLi initiated polybutadiene terminated by MeOD (61 MHz, chloroform-*d*).

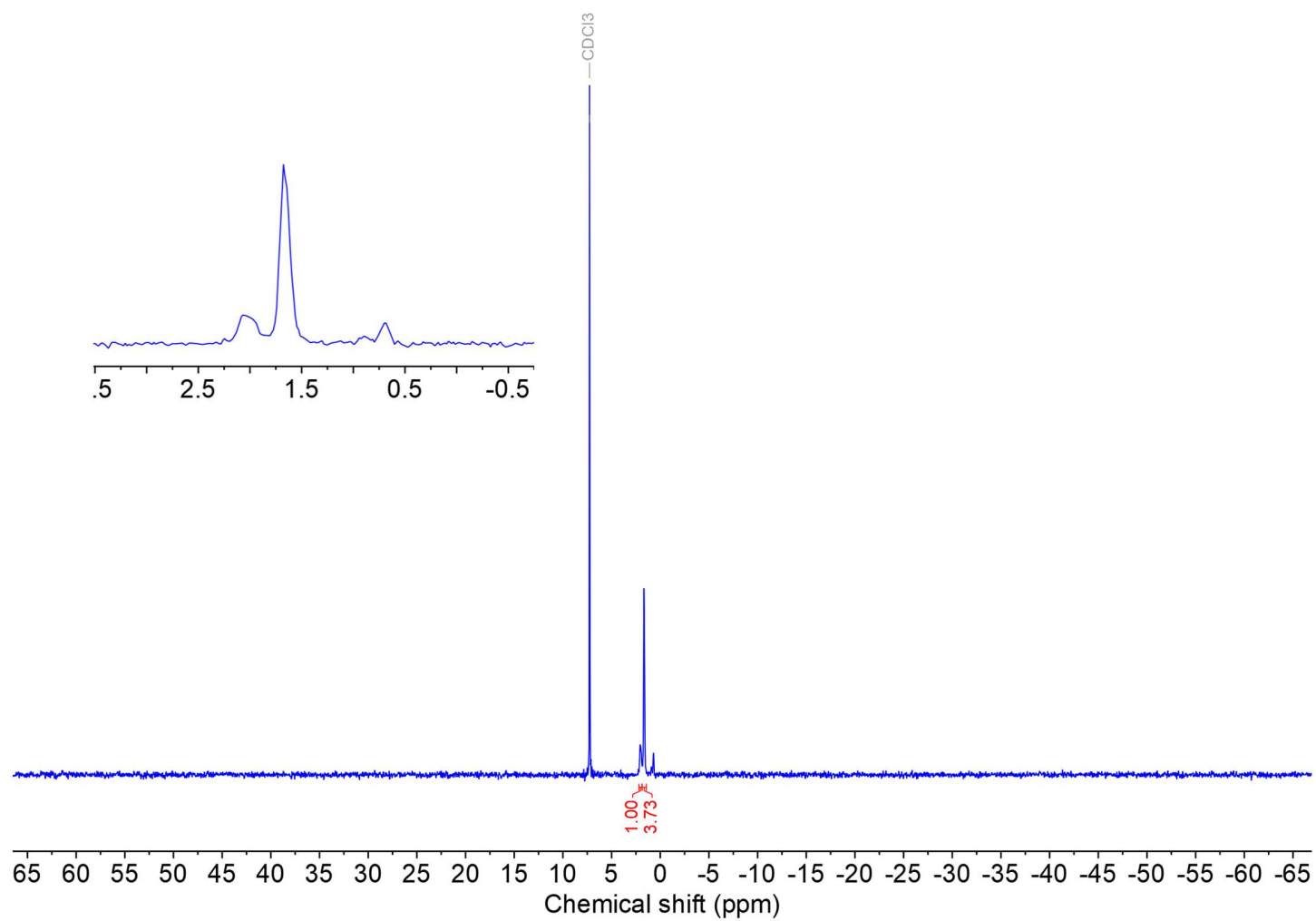


Figure S51. ^2H NMR spectrum of **5** DiPyr/n-BuLi initiated polybutadiene terminated by MeOD (61 MHz, chloroform-d).

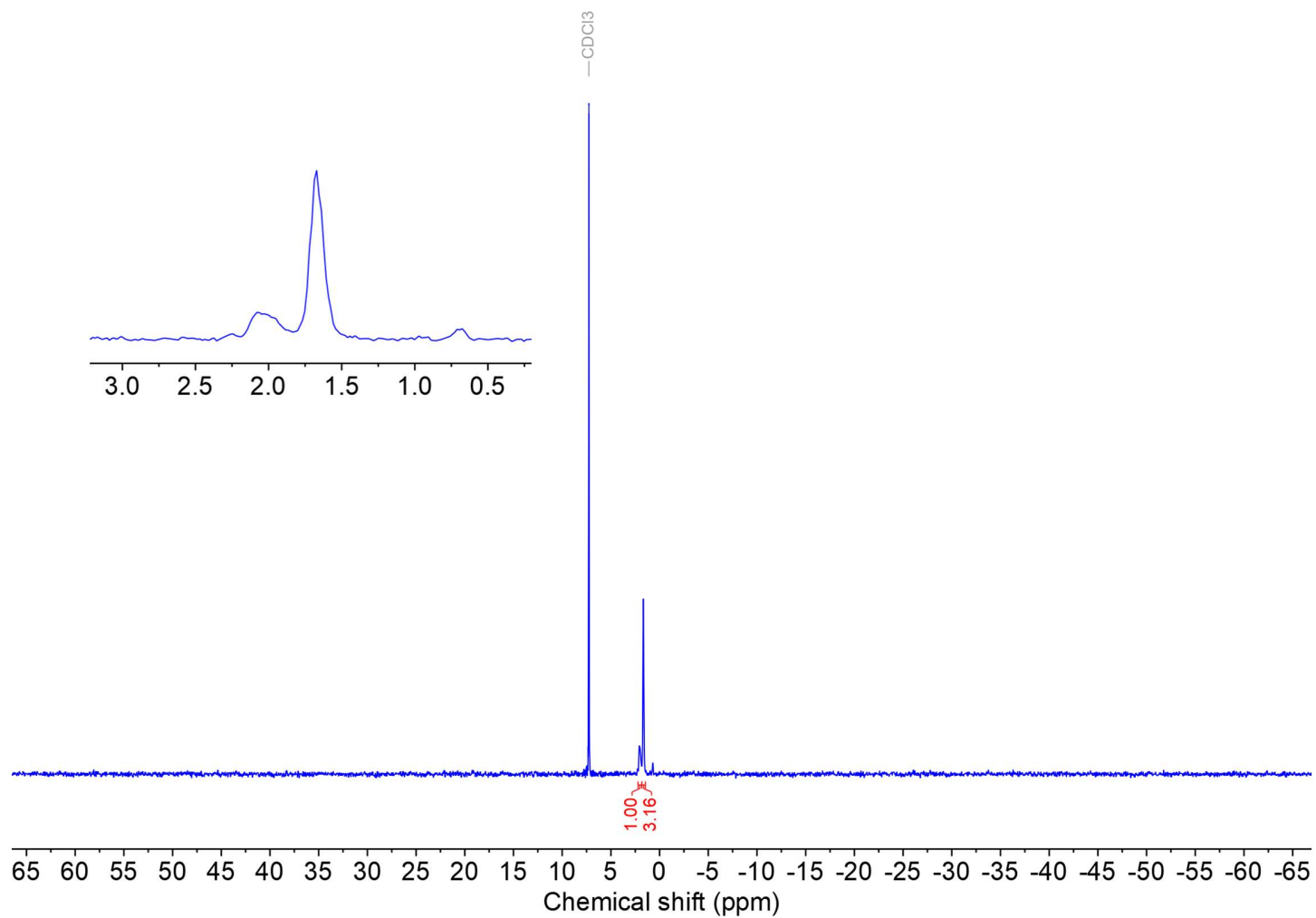


Figure S52. ^2H NMR spectrum of **6** DiPip/n-BuLi initiated polybutadiene terminated by MeOD (61 MHz, chloroform-d).

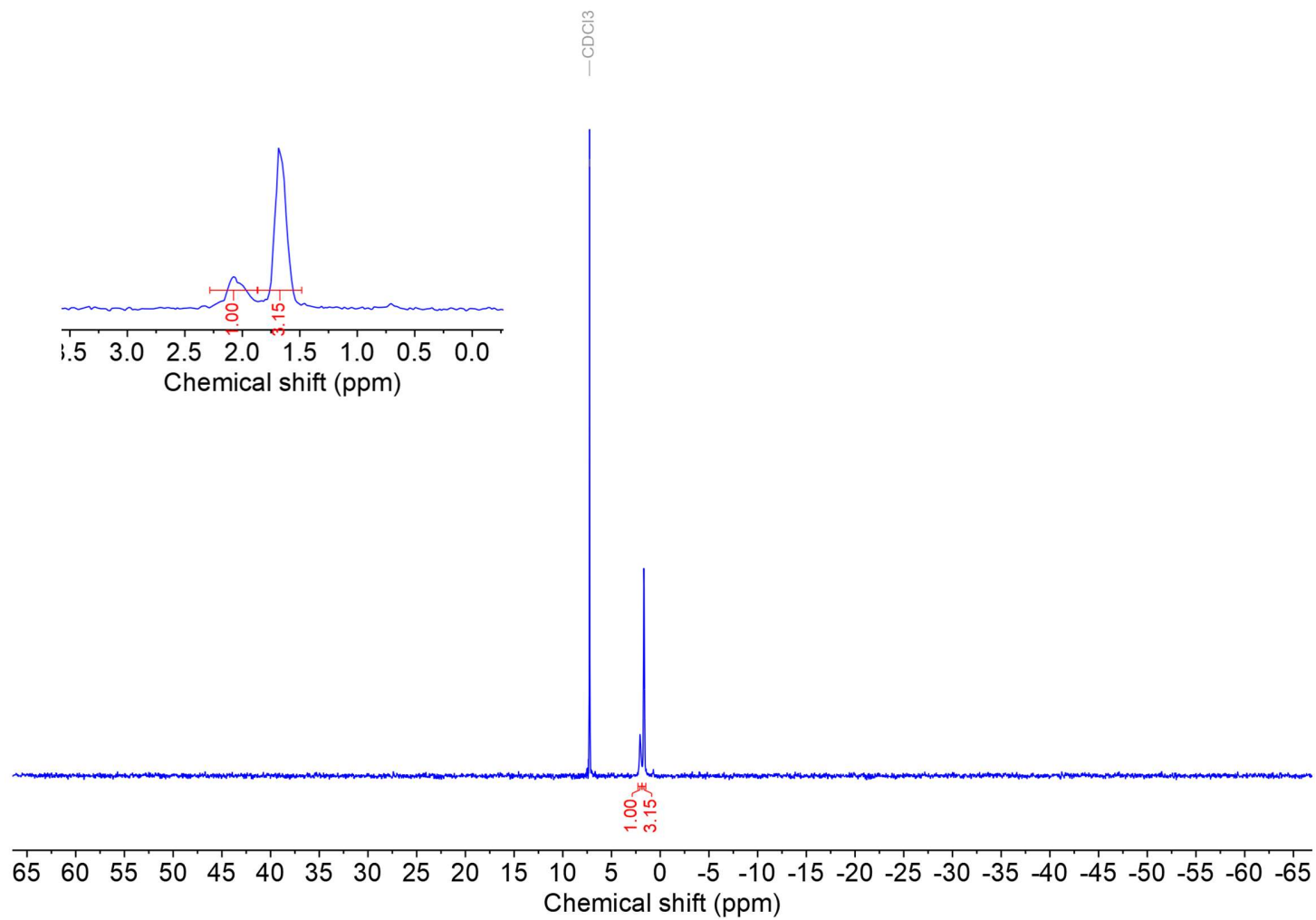


Figure S53. ^2H NMR spectrum of 7 DiAze/n-BuLi initiated polybutadiene terminated by MeOD (61 MHz, chloroform-d).

Spectroscopic Data — ^{13}C NMR Spectra of Lewis Bases/*n*-BuLi Initiated Polybutadiene Terminated by MeOD

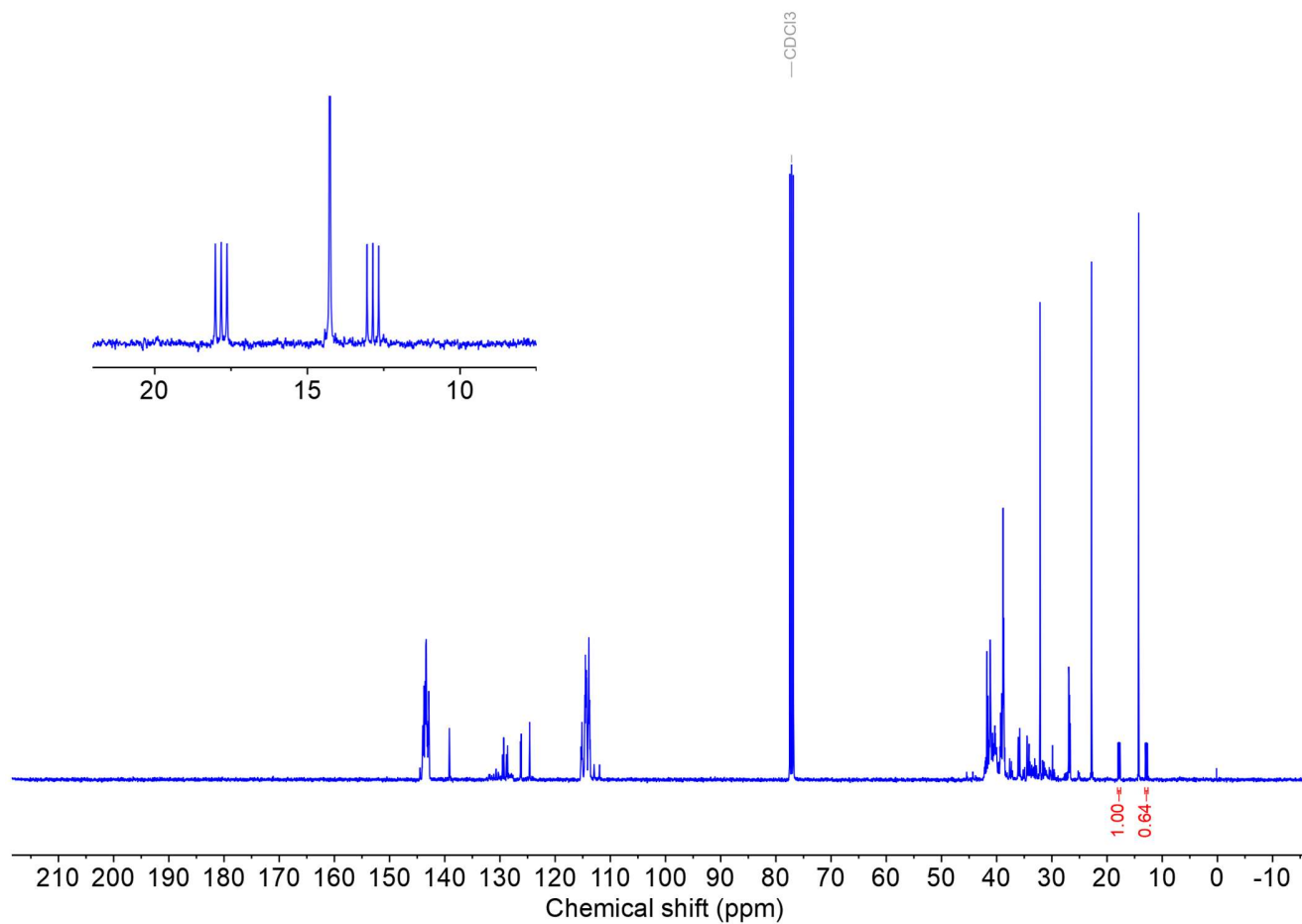


Figure S54. ^{13}C NMR spectrum of **1** glyme/*n*-BuLi initiated polybutadiene terminated by MeOD (61 MHz, chloroform-d).

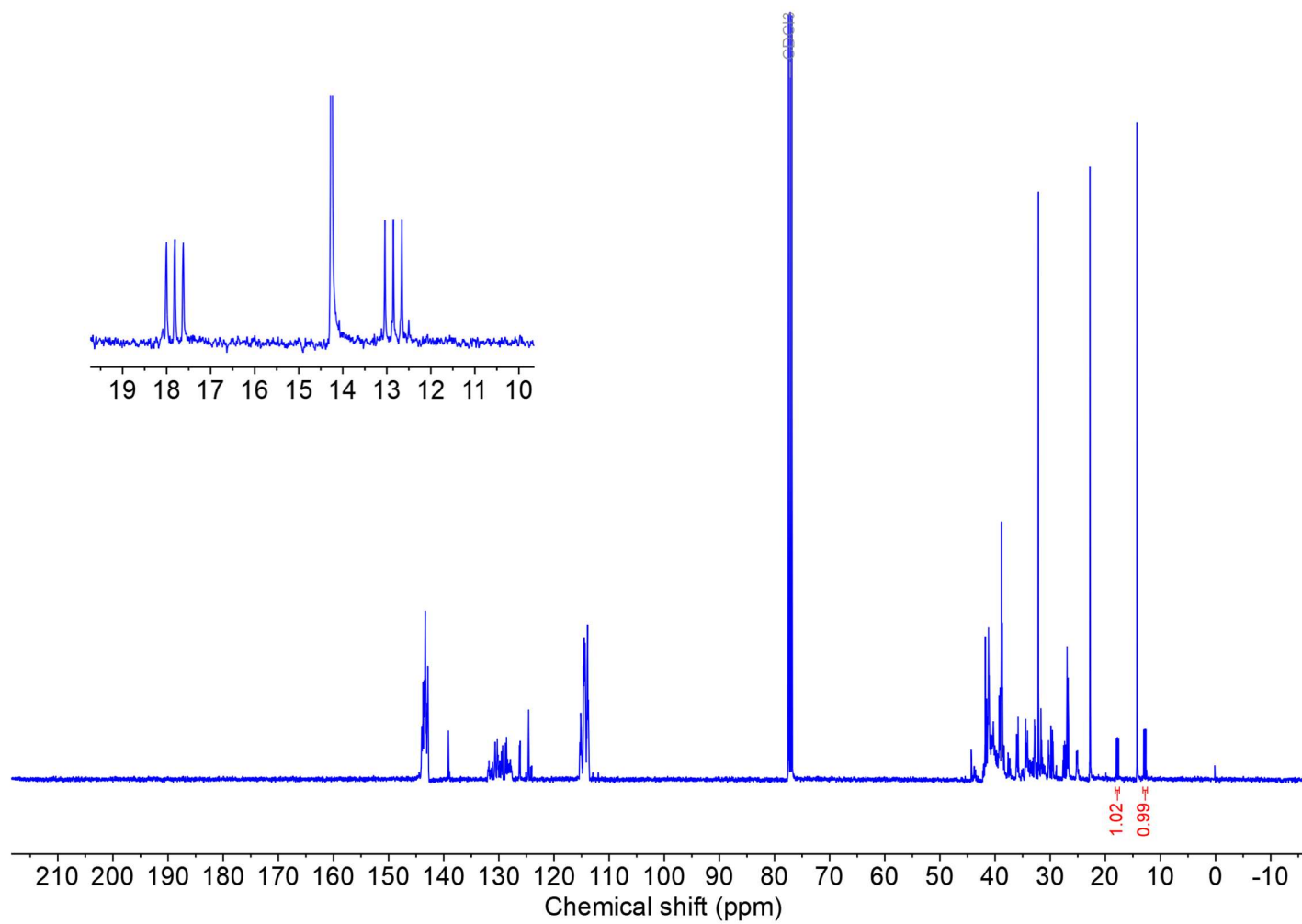


Figure S55. ^{13}C NMR spectrum of **2** THF/*n*-BuLi initiated polybutadiene terminated by MeOD (61 MHz, chloroform-*d*).

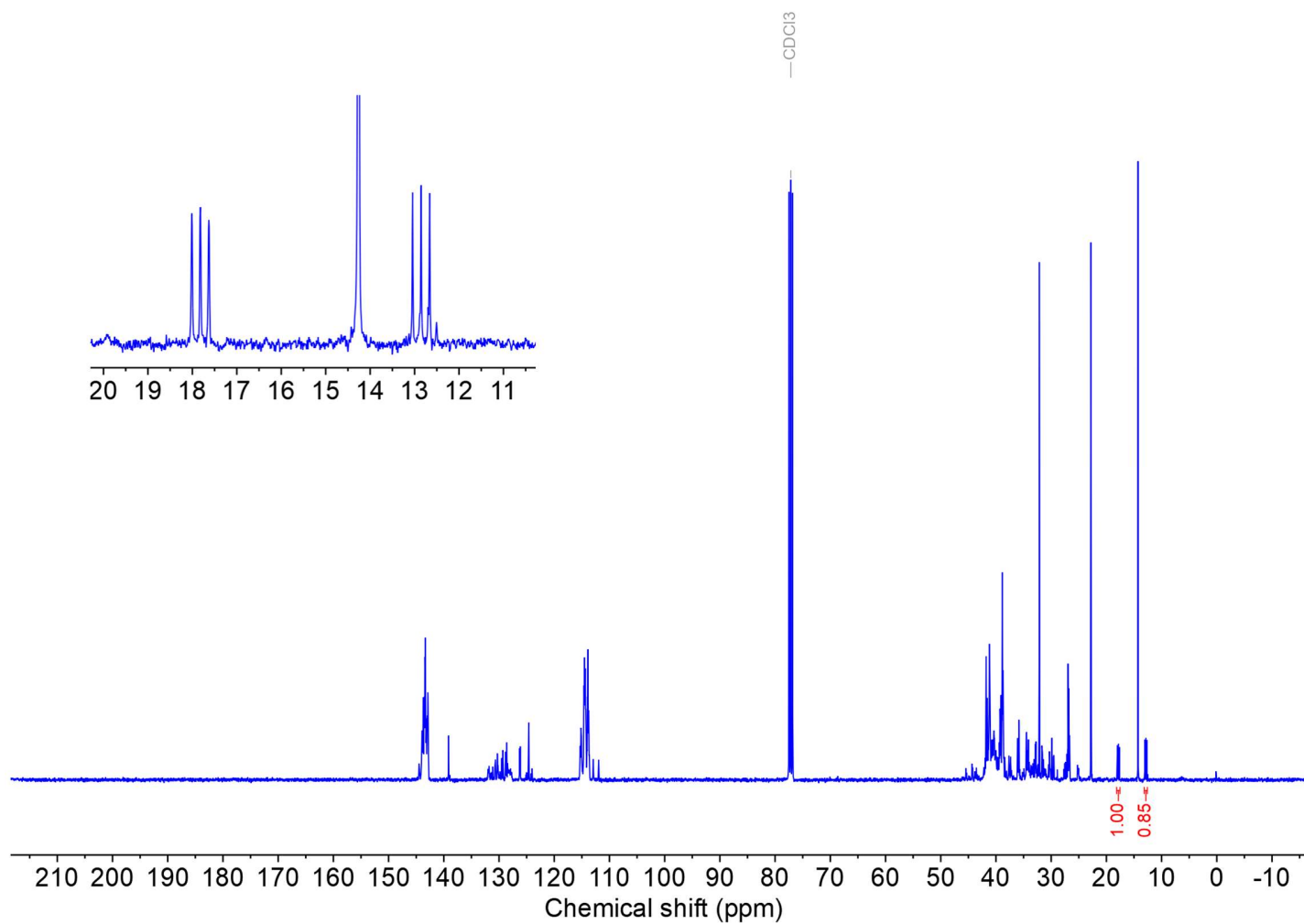


Figure S56. ^{13}C NMR spectrum of **3** TMEDA/*n*-BuLi initiated polybutadiene terminated by MeOD (61 MHz, chloroform-*d*).

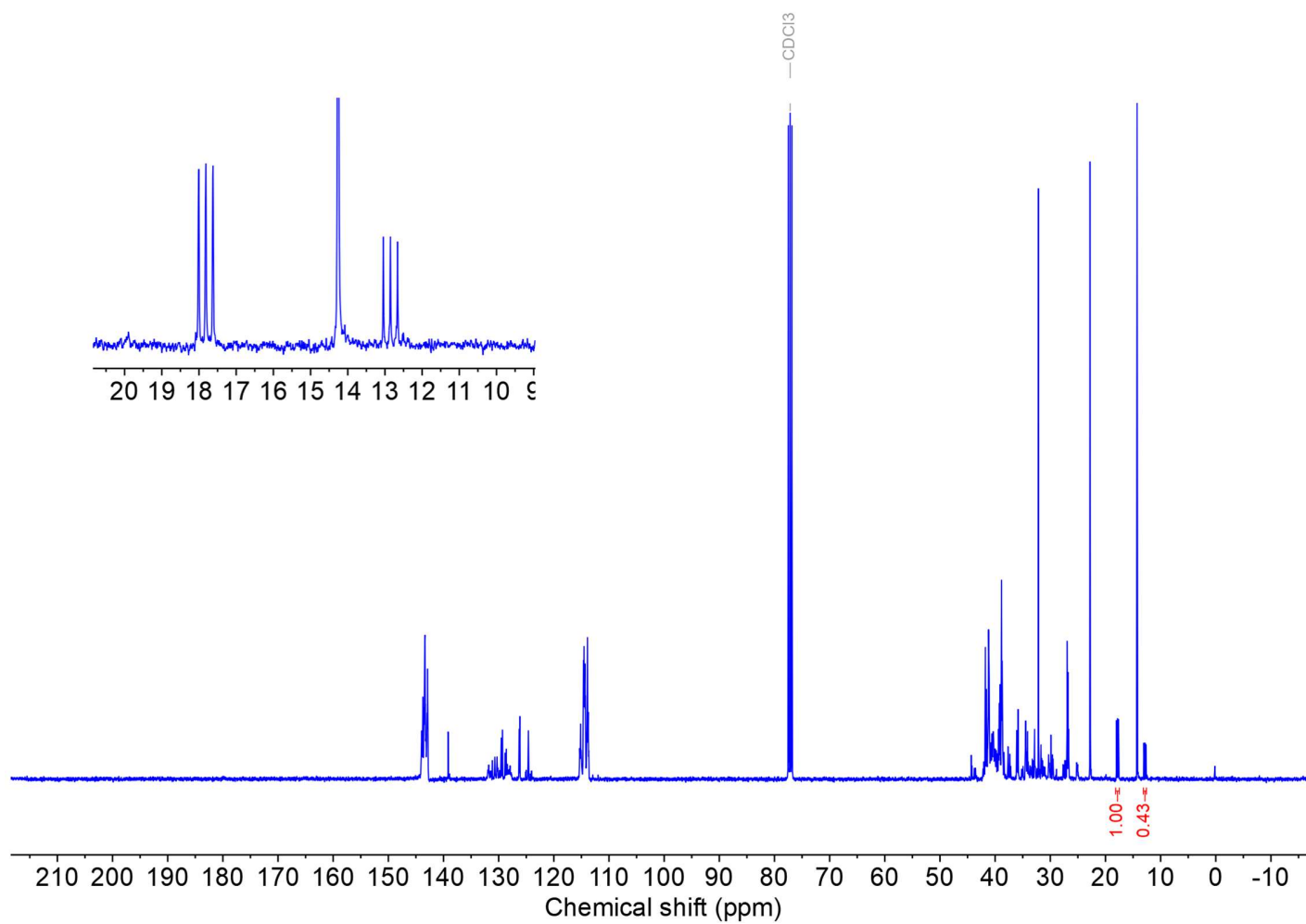


Figure S57. ^{13}C NMR spectrum of **4** TEEDA/*n*-BuLi initiated polybutadiene terminated by MeOD (61 MHz, chloroform-*d*).

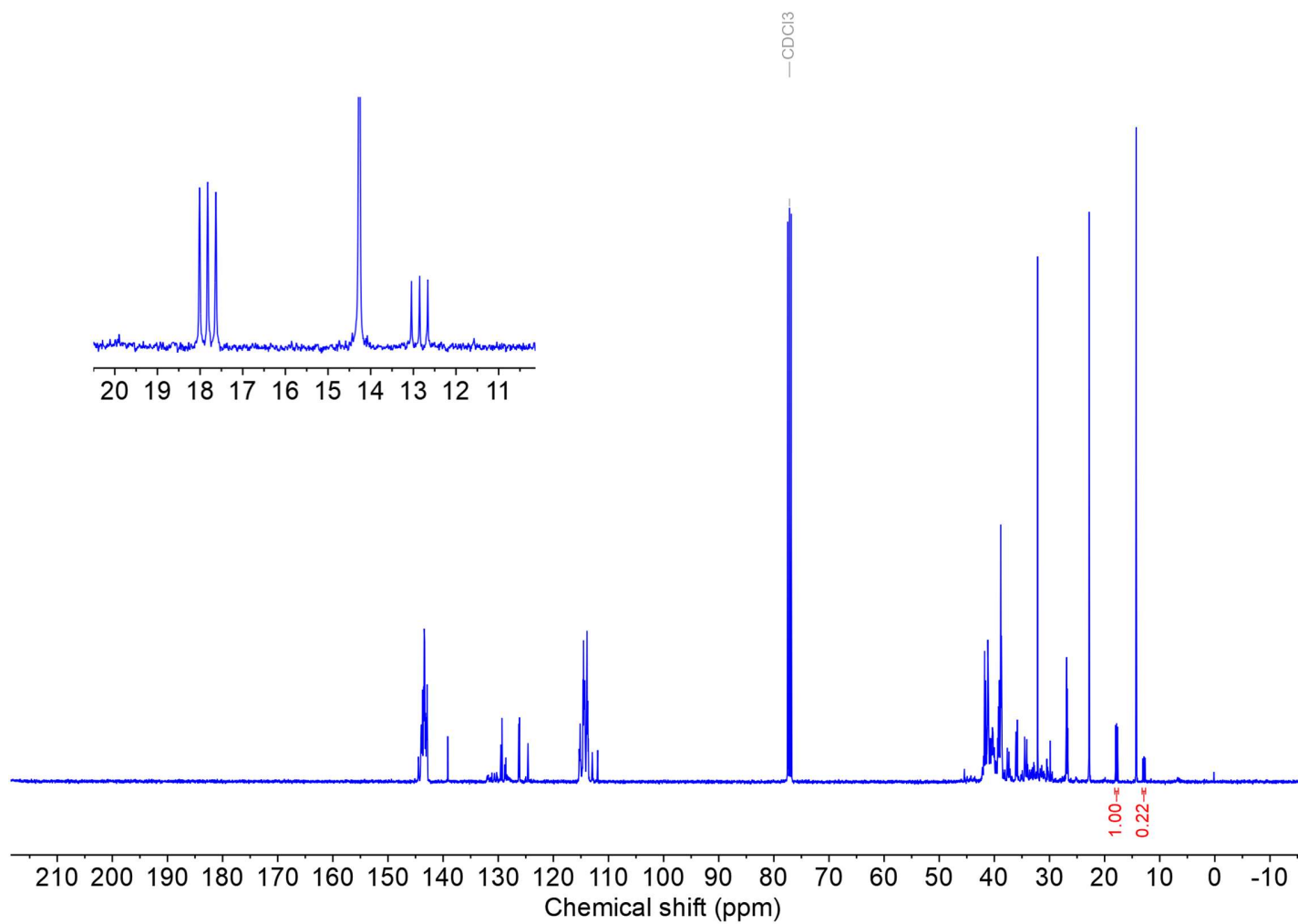


Figure S58. ^{13}C NMR spectrum of **5** DiPyr/n-BuLi initiated polybutadiene terminated by MeOD (61 MHz, chloroform-d).

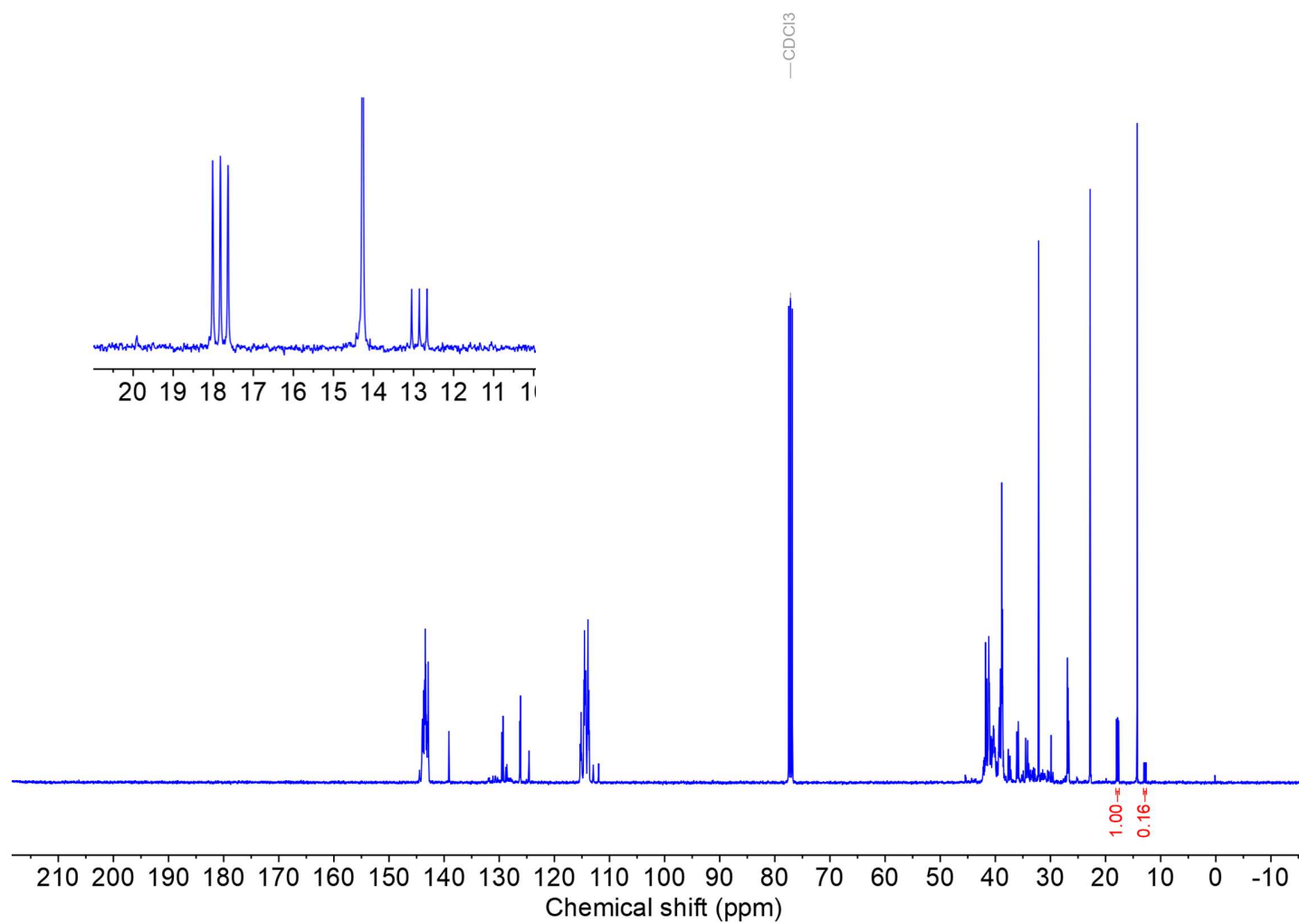


Figure S59. ^{13}C NMR spectrum of **6** DiPip/n-BuLi initiated polybutadiene terminated by MeOD (61 MHz, chloroform-d).

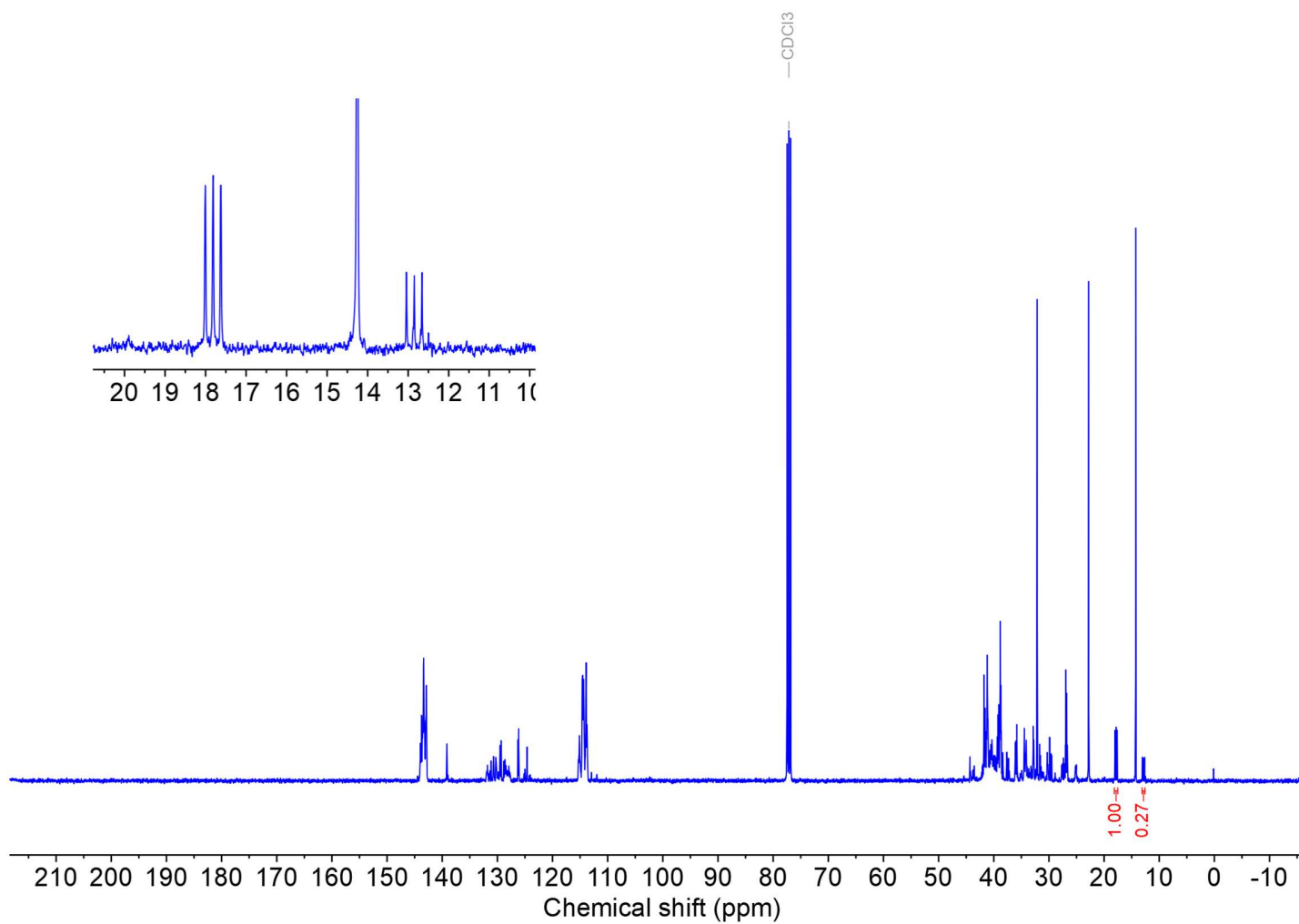


Figure S60. ^{13}C NMR spectrum of **7** DiAze/n-BuLi initiated polybutadiene terminated by MeOD (61 MHz, chloroform-d).

Spectroscopic Data — FTIR Spectra of the Polybutadiene

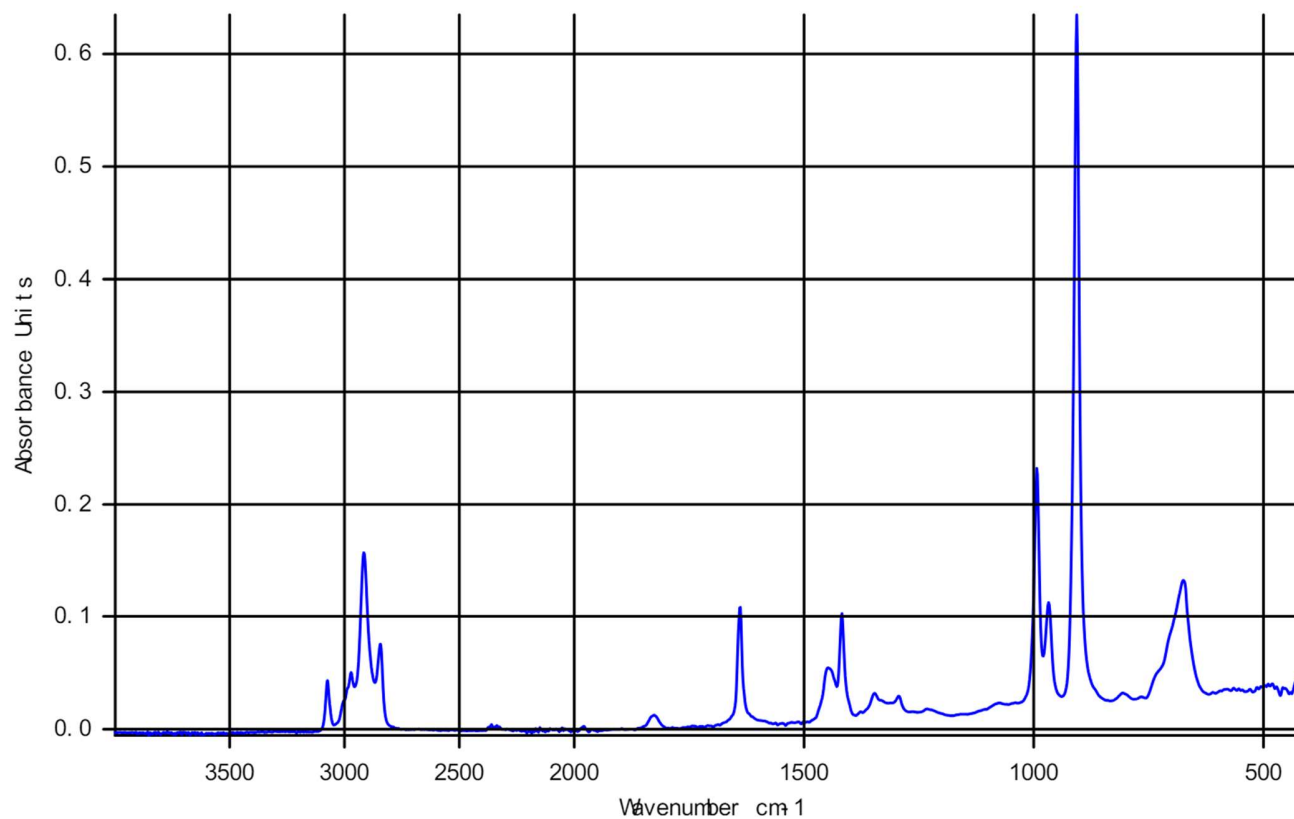


Figure S61. FTIR spectrum of polybutadiene in entry 1 of Table 1 (**1** glyme as ligand).

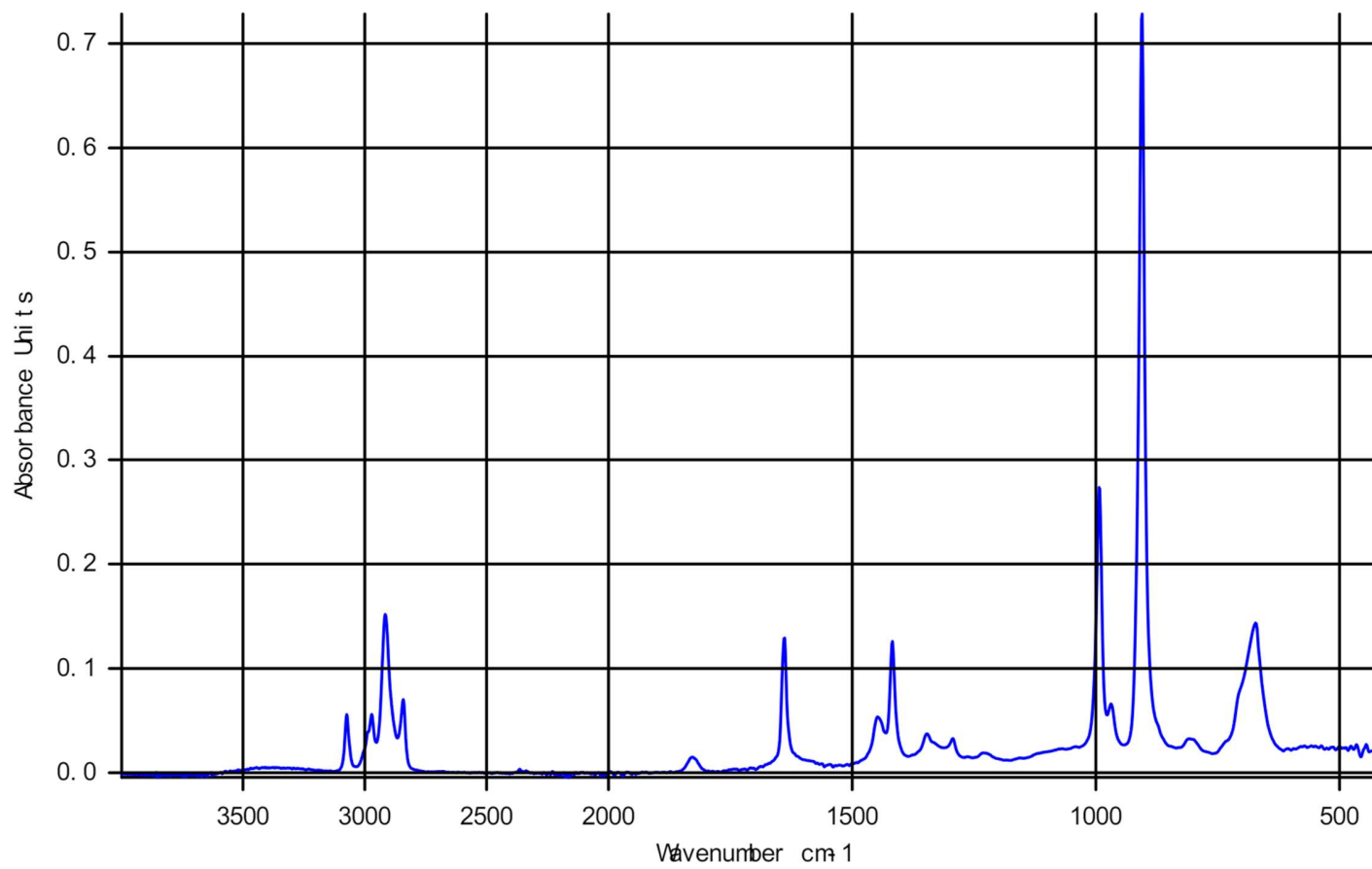


Figure S62. FTIR spectrum of polybutadiene in entry 2 of Table 1 (**2** THF as ligand).

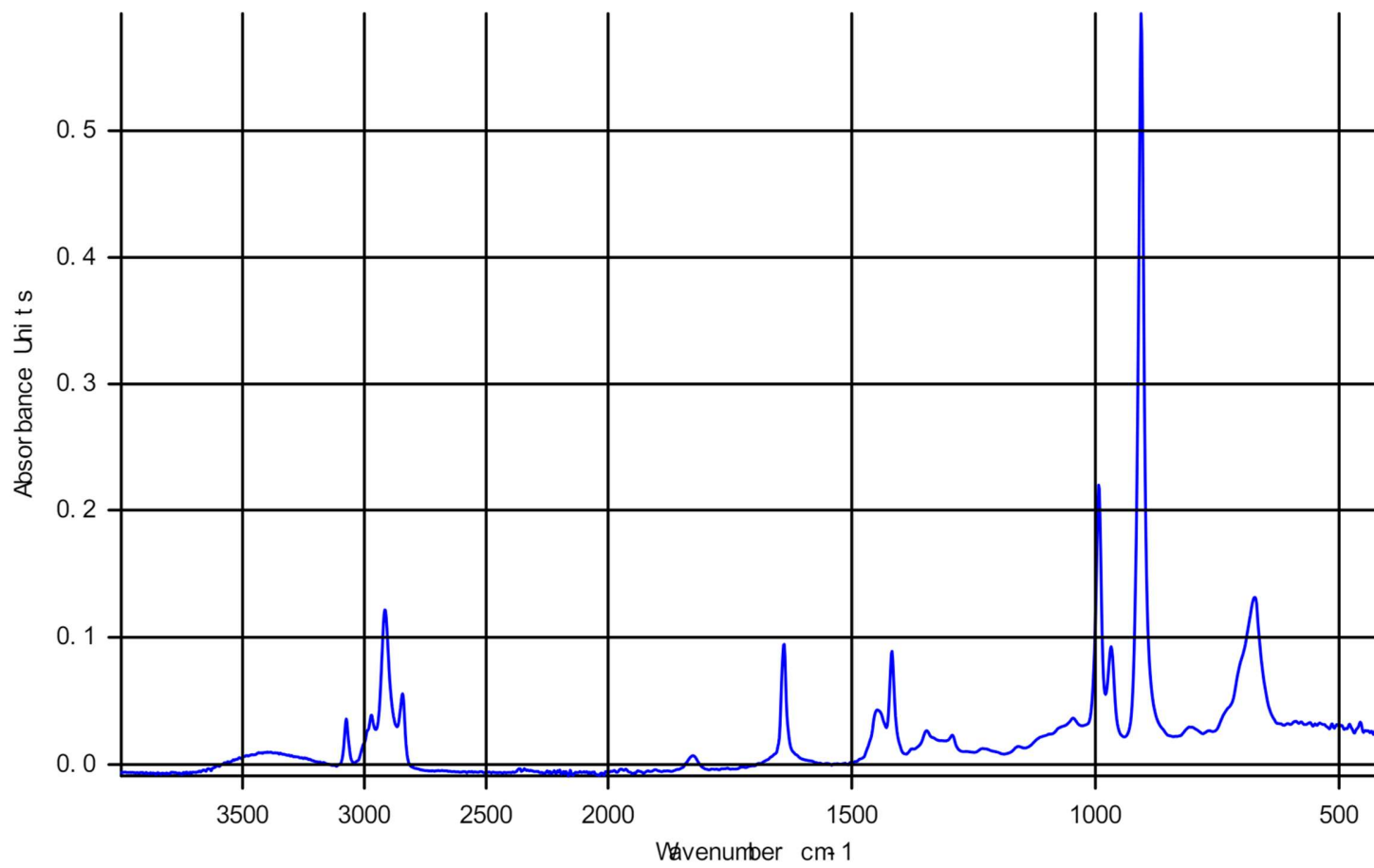


Figure S63. FTIR spectrum of polybutadiene in entry 3 of Table 1 (**3** TMEDA as ligand).

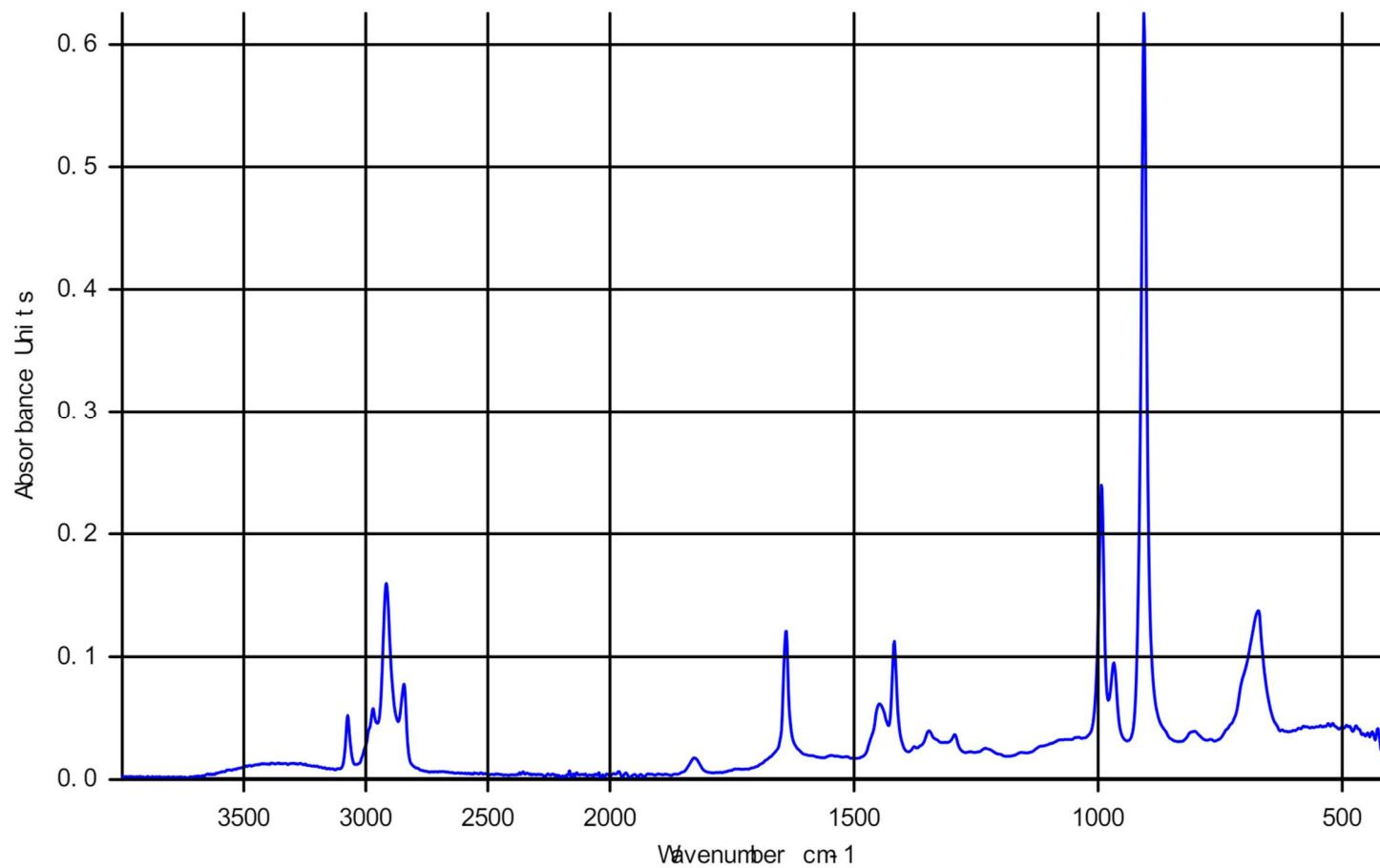


Figure S64. FTIR spectrum of polybutadiene in entry 4 of Table 1 (**4** TEEDA as ligand).

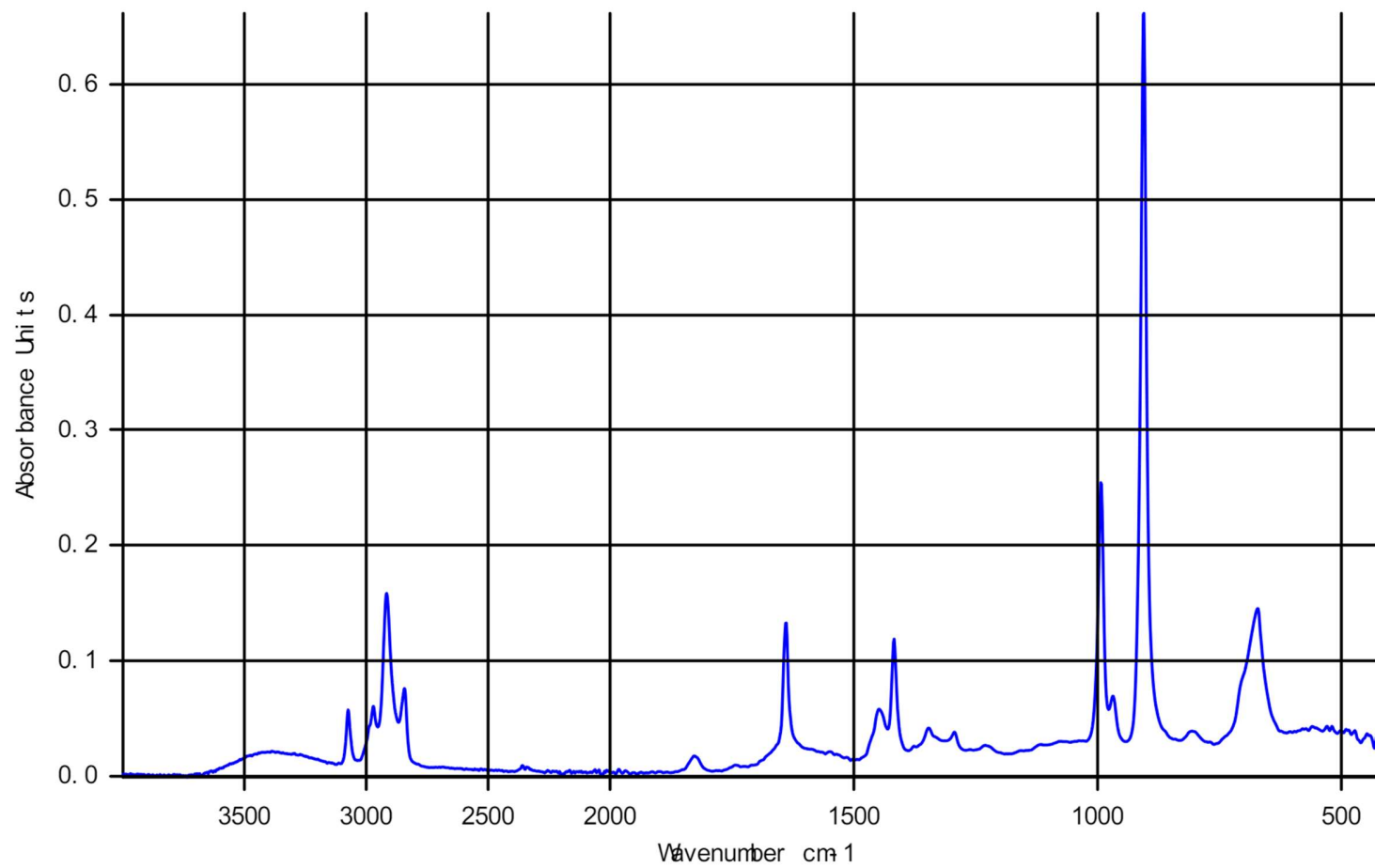


Figure S65. FTIR spectrum of polybutadiene in entry 5 of Table 1 (5 DiPyr as ligand).

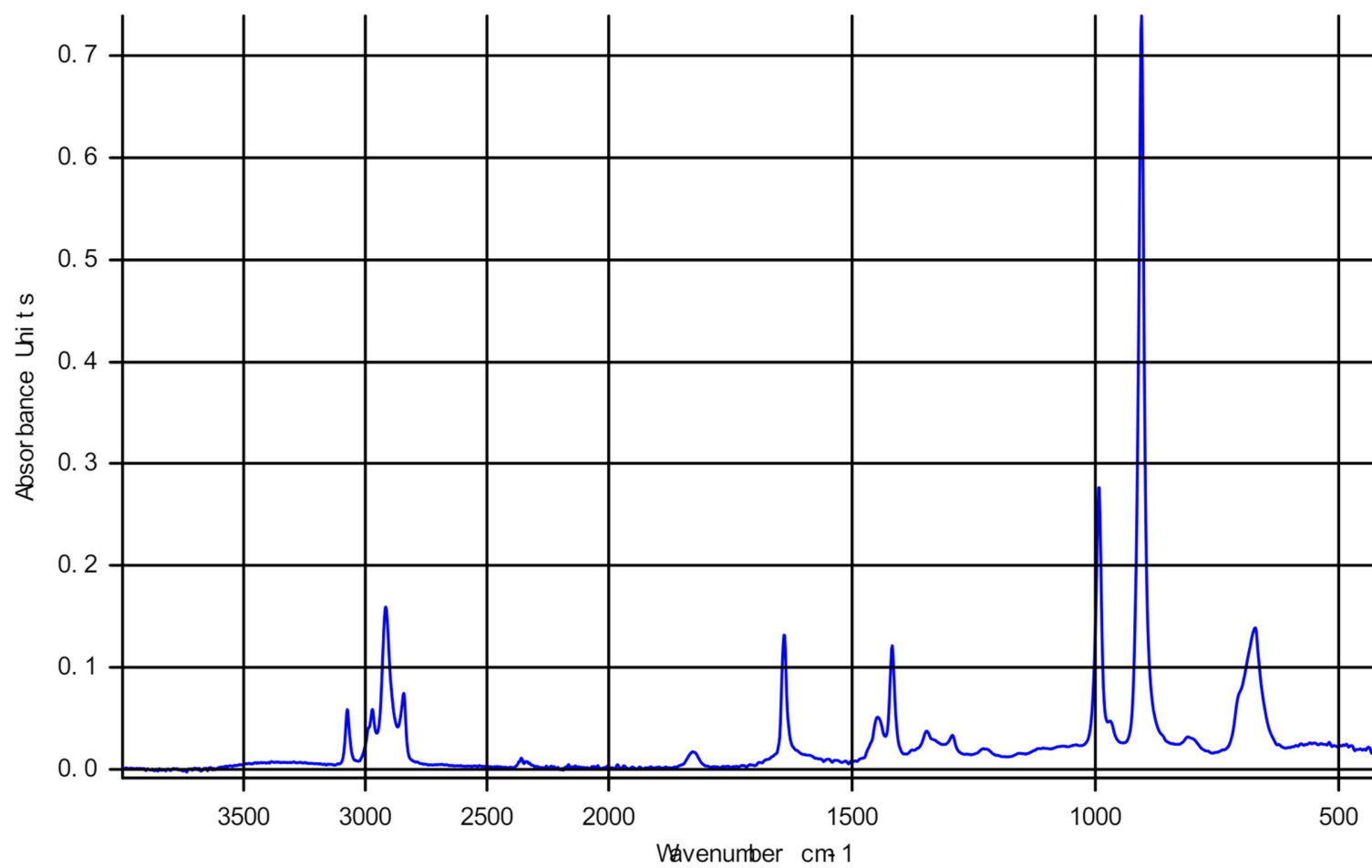


Figure S66. FTIR spectrum of polybutadiene in entry 6 of Table 1 (6 DiPip as ligand).

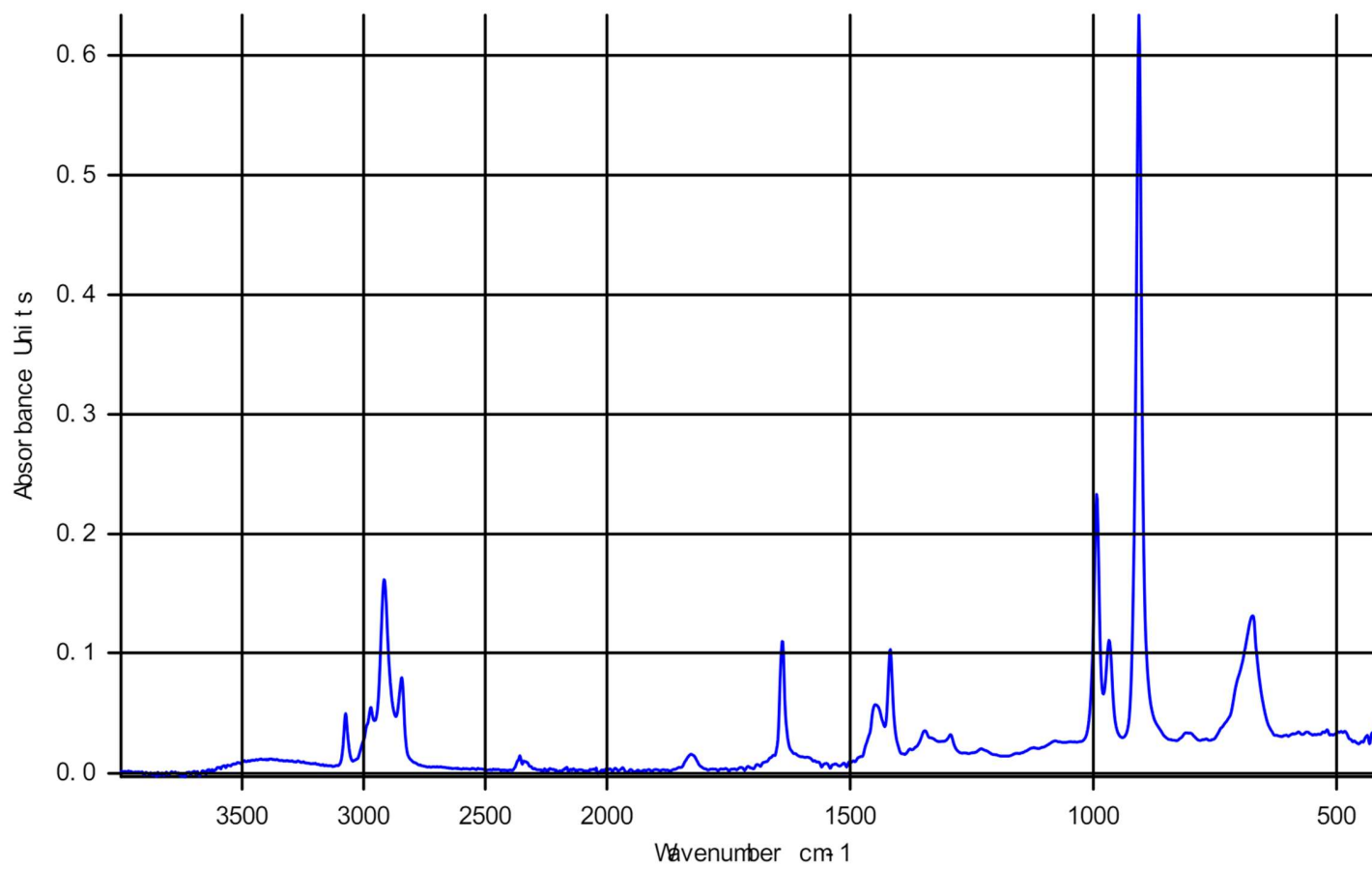


Figure S67. FTIR spectrum of polybutadiene in entry 7 of Table 1 (**7** DiAze as ligand).

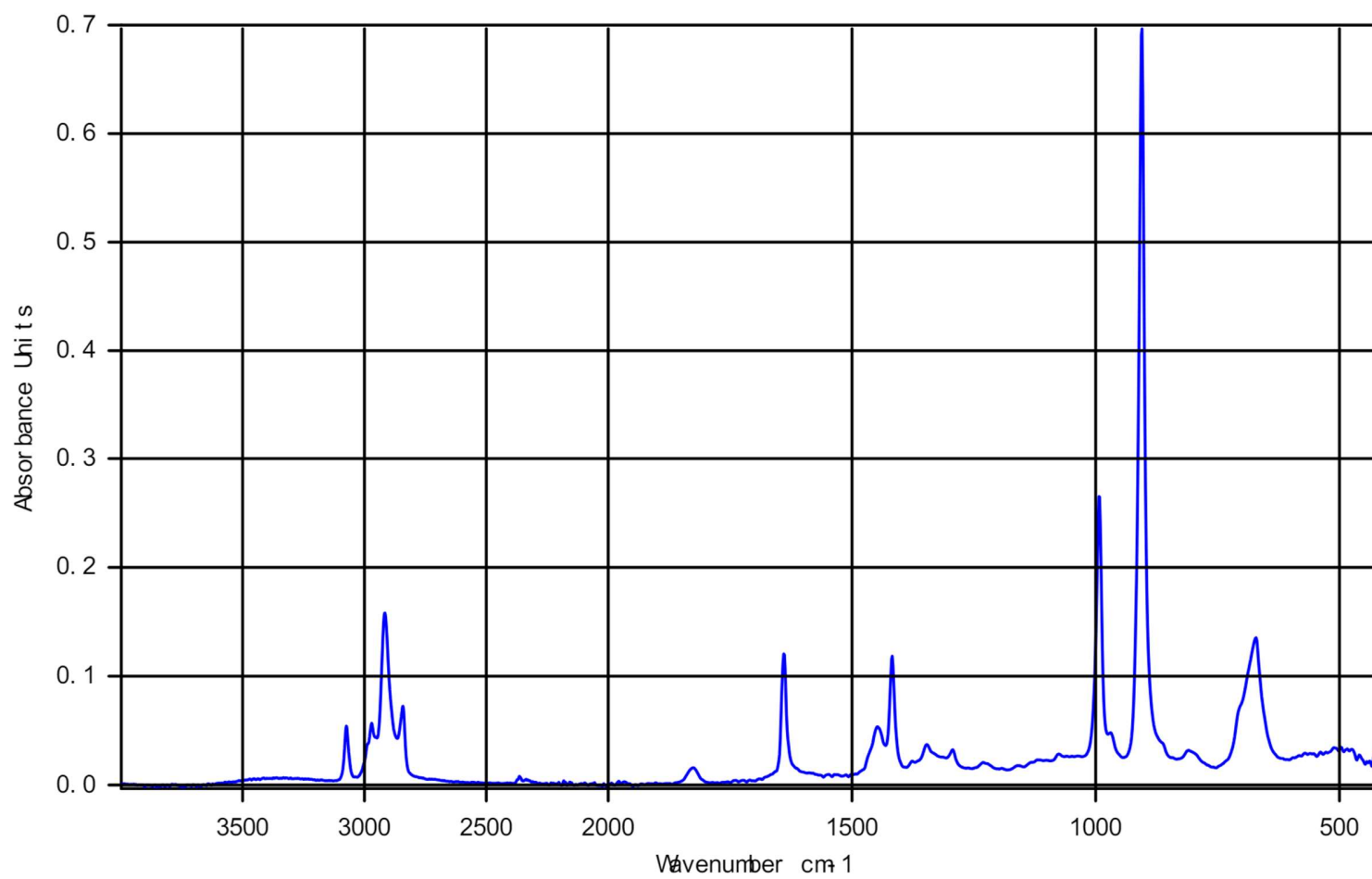


Figure S68. FTIR spectrum of polybutadiene (**8** MeDiPip as ligand).

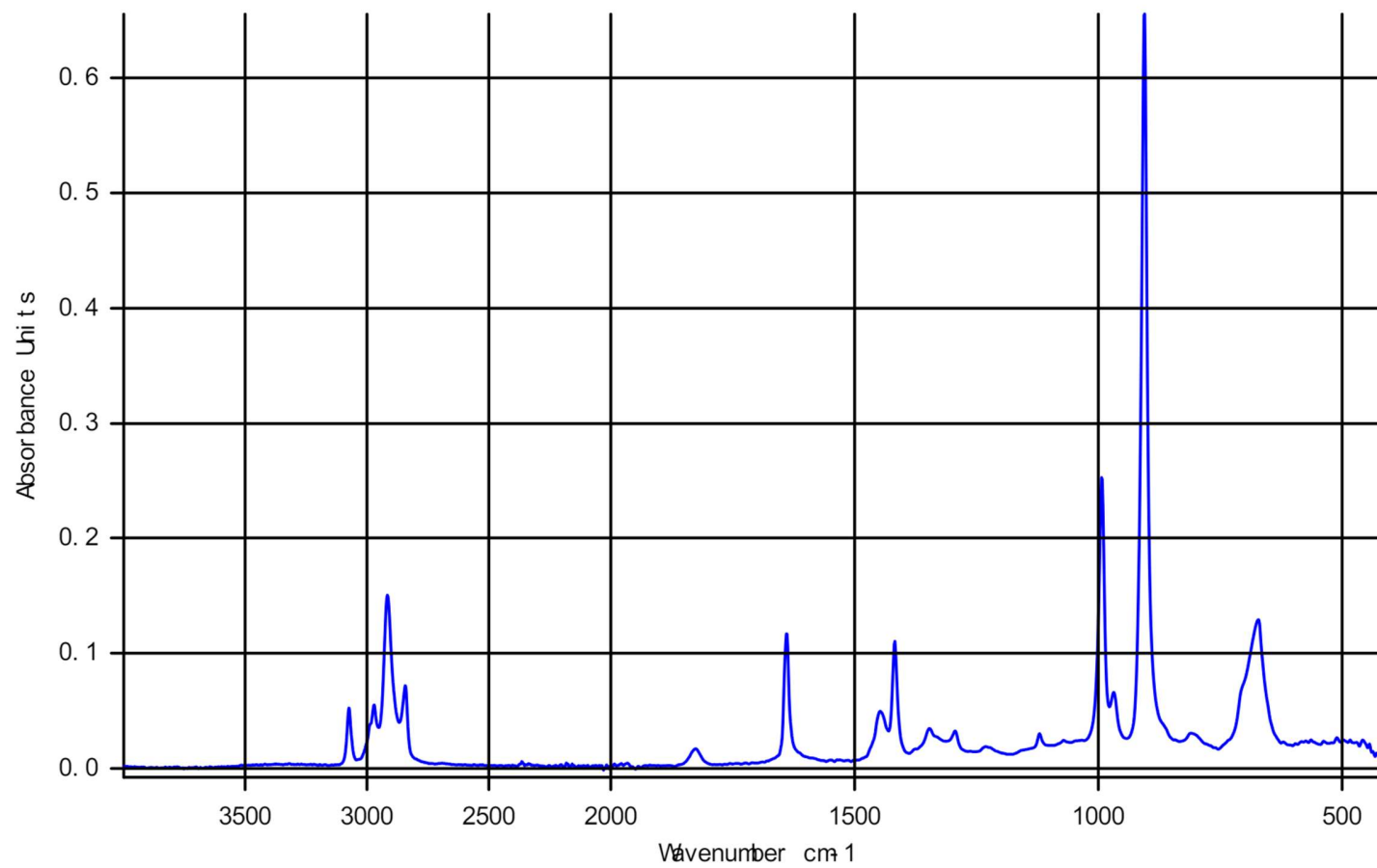


Figure S69. FTIR spectrum of polybutadiene (**9** DiMph as ligand).

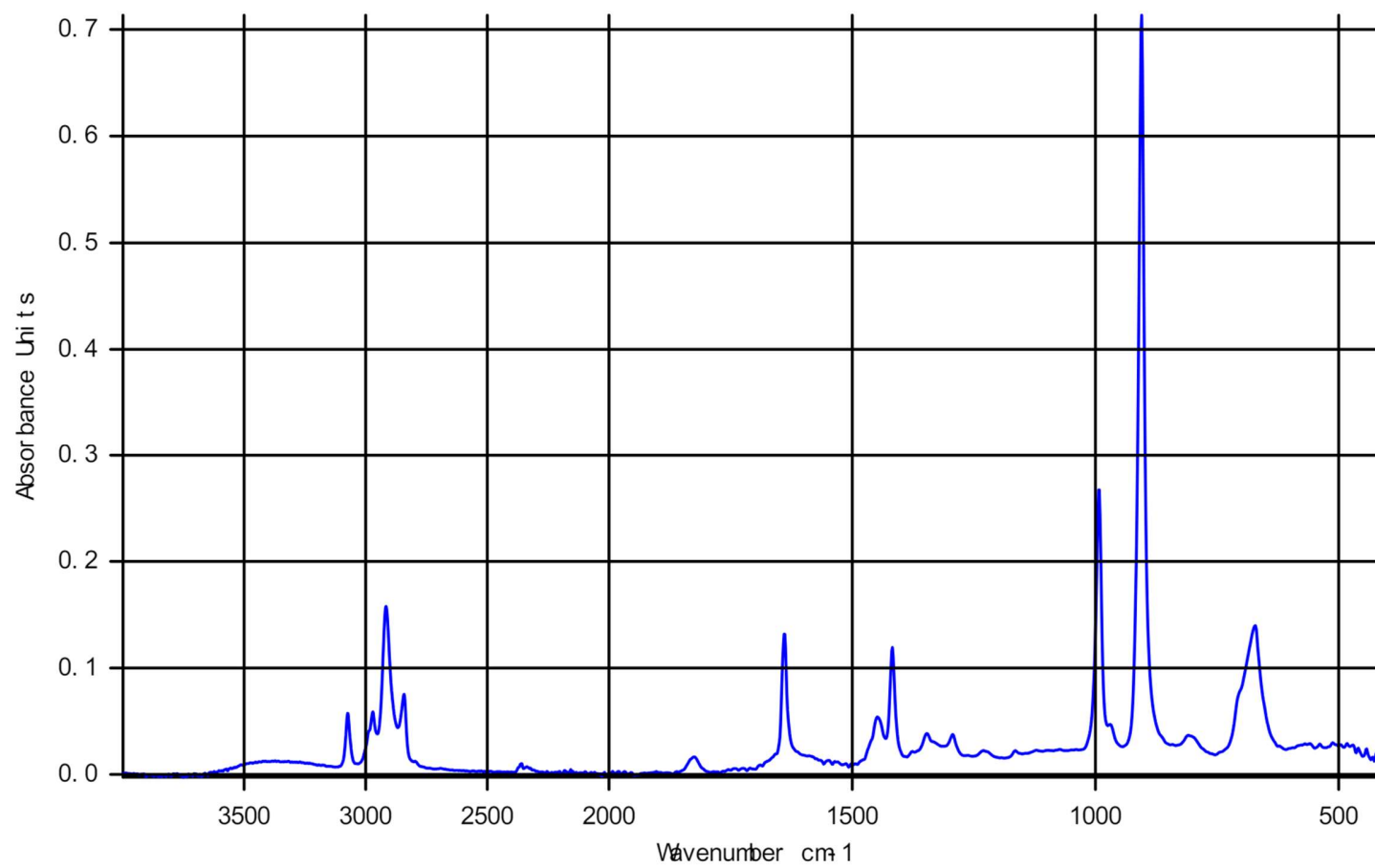


Figure S70. FTIR spectrum of polybutadiene (**10** MeDiPz as ligand).

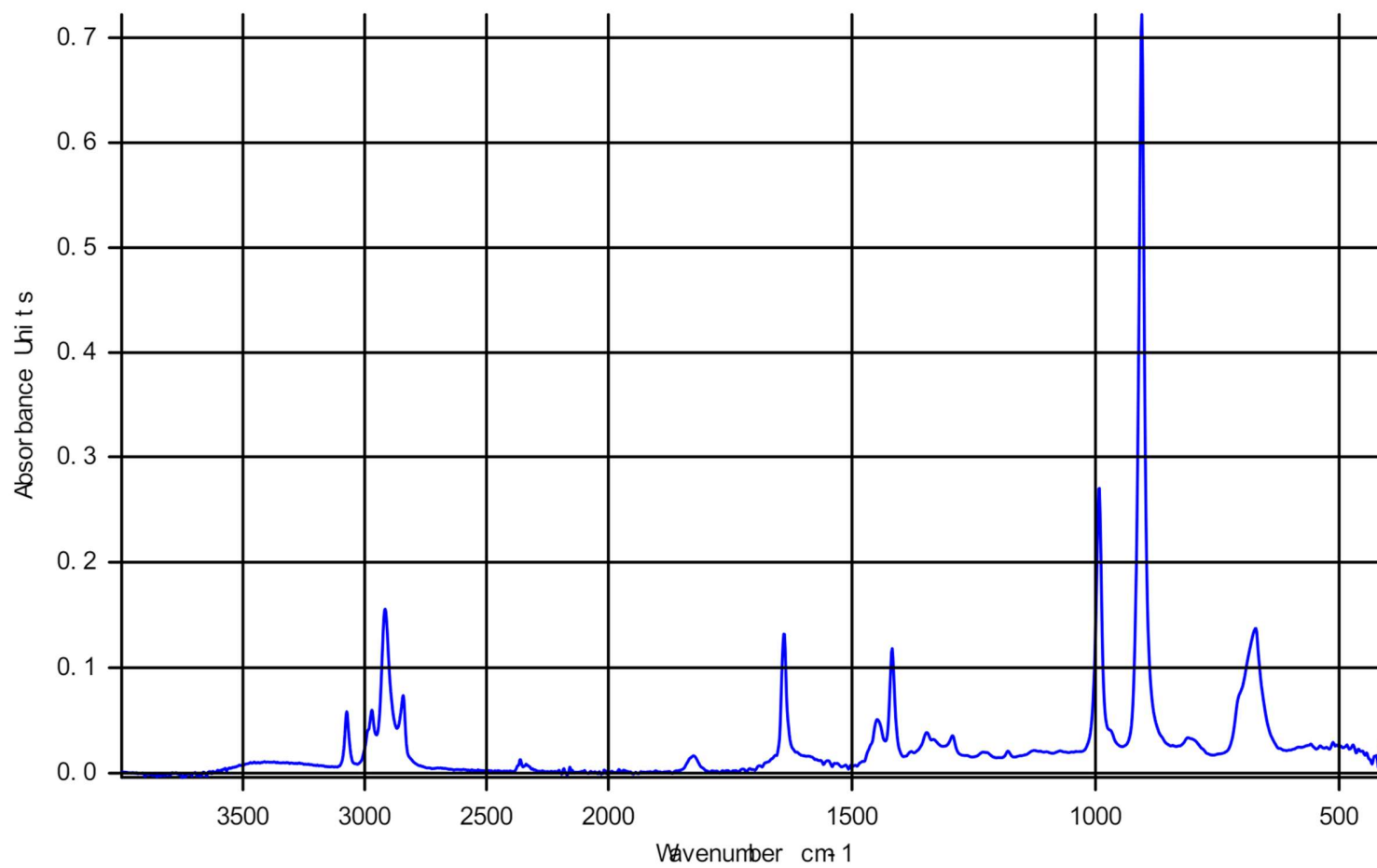


Figure S71. FTIR spectrum of polybutadiene (11 iPrDiPz as ligand).

Spectroscopic Data — ^1H , ^{13}C NMR Spectra of the Polybutadiene

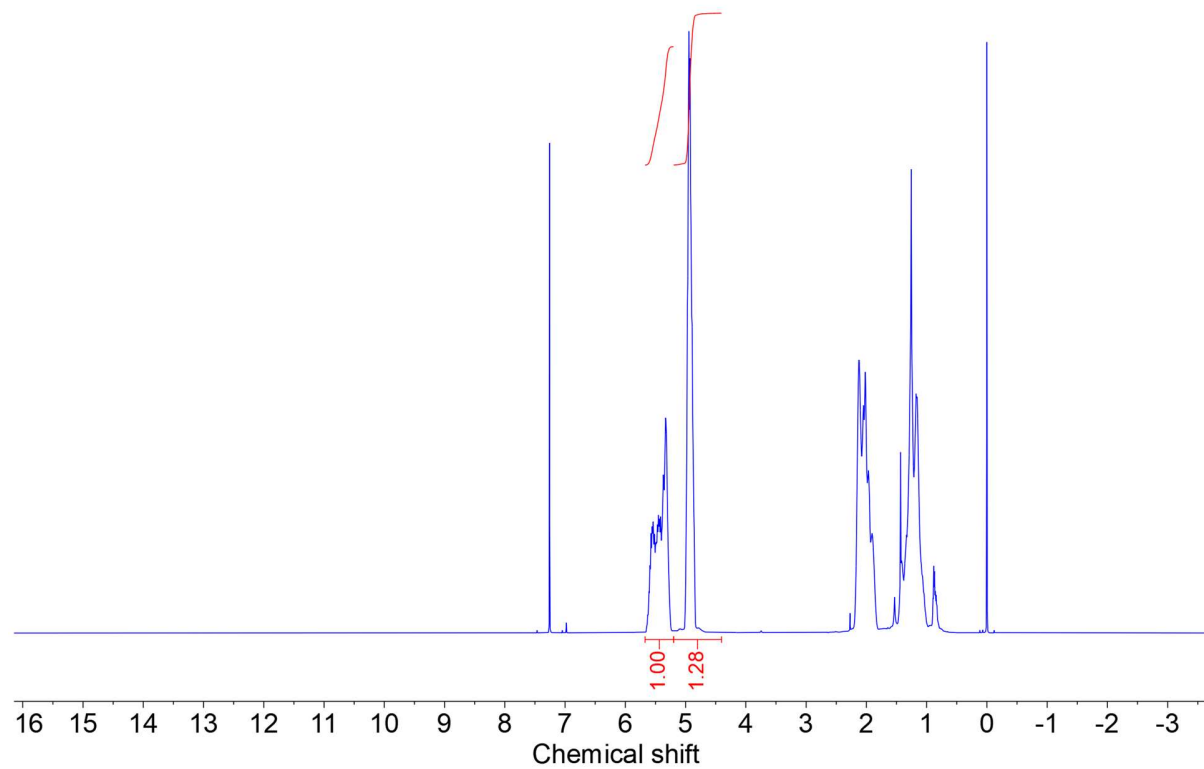


Figure S72. ^1H NMR spectrum of polybutadiene in entry 1 of Table 1 (1 glyme as ligand, polymerization at 20°C. 500 MHz, chloroform-d).

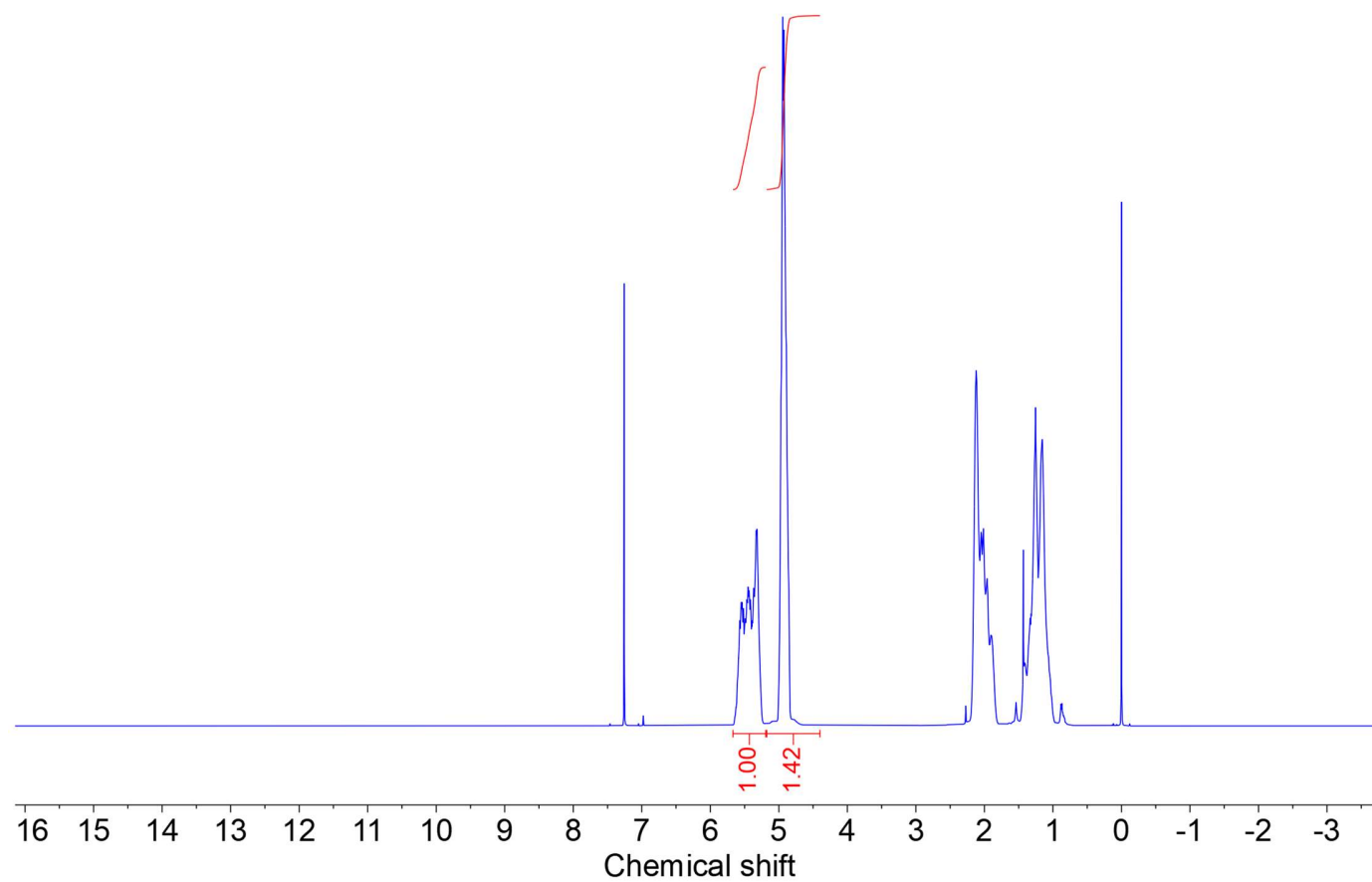


Figure S73. ^1H NMR spectrum of polybutadiene (**1** glyme as ligand, polymerization at 0°C . 500 MHz, chloroform-d).

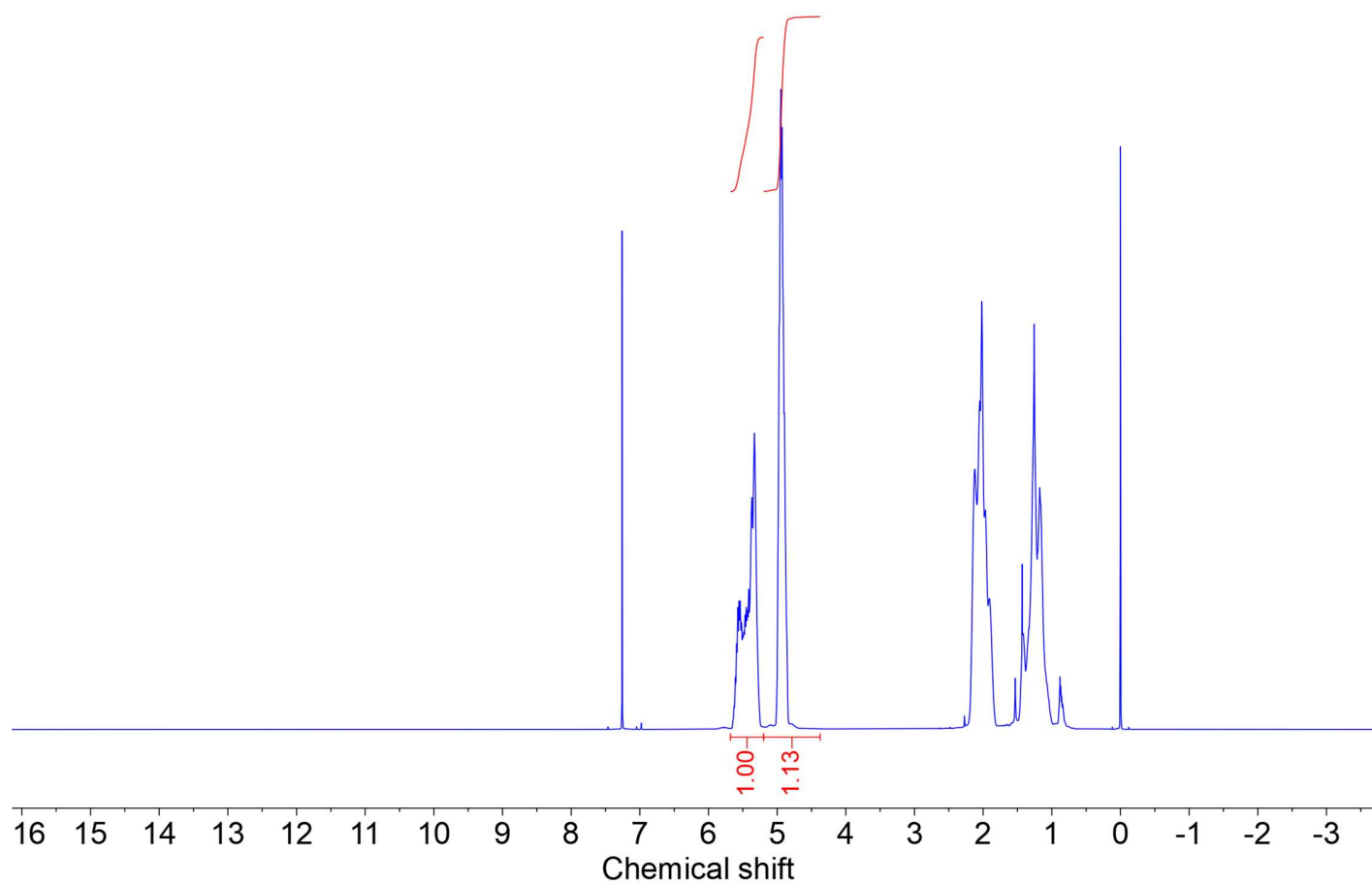


Figure S74. ^1H NMR spectrum of polybutadiene (1 glyme as ligand, polymerization at 40°C. 500 MHz, chloroform-d).

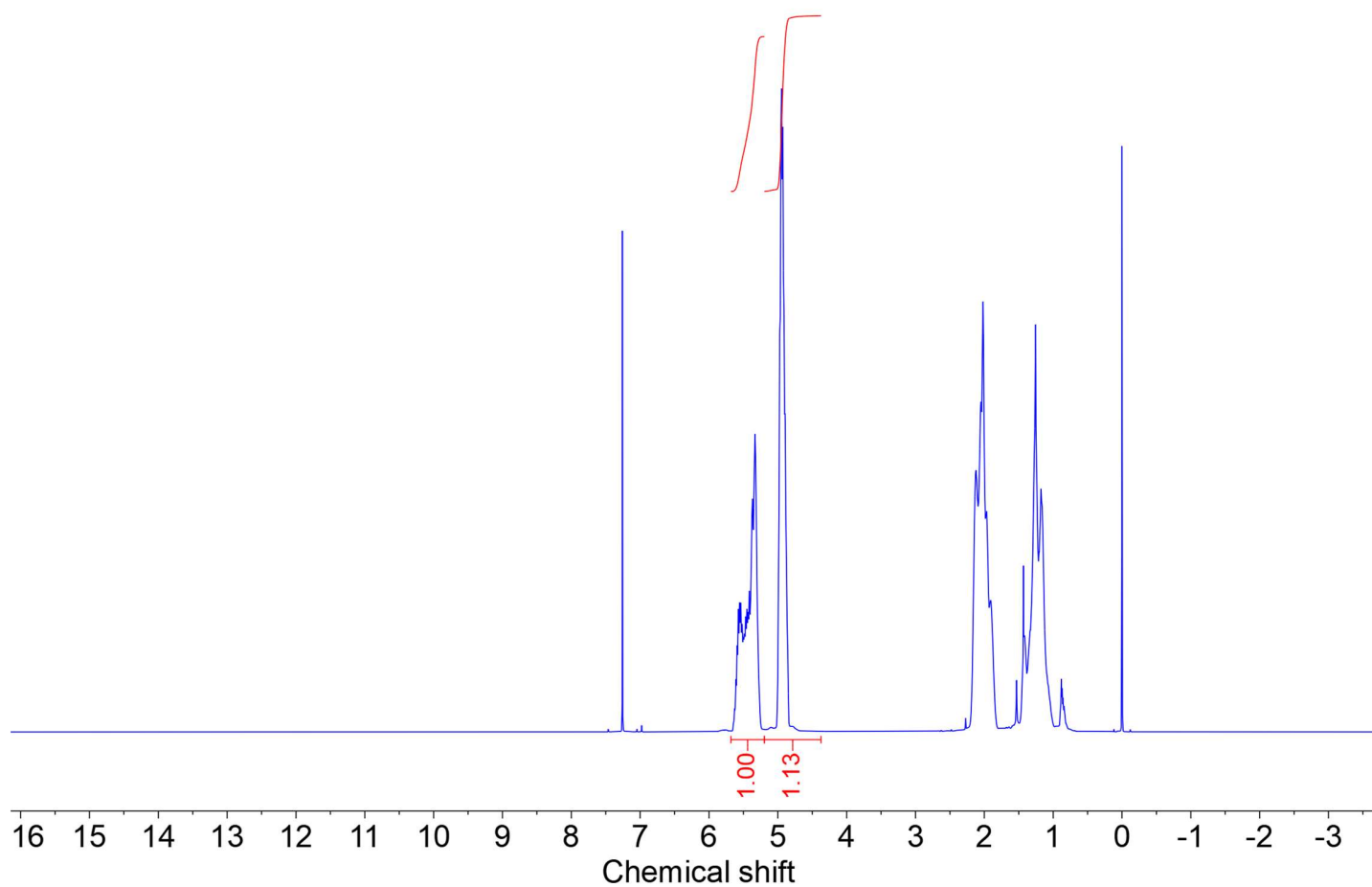


Figure S75. ^1H NMR spectrum of polybutadiene (1 glyme as ligand, polymerization at 60°C. 500 MHz, chloroform-d).

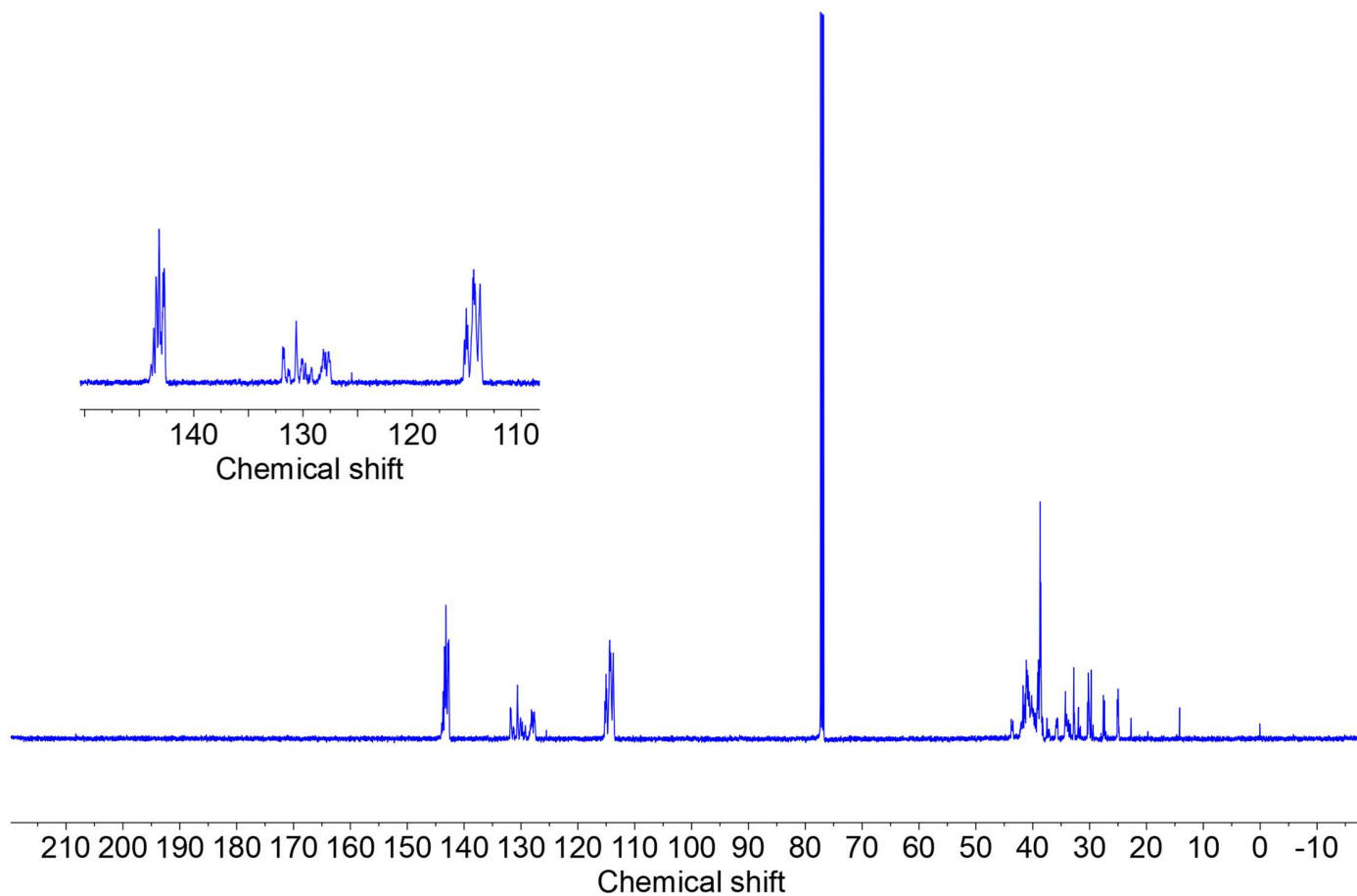


Figure S76. ^{13}C NMR spectrum of polybutadiene in entry 1 of Table 1 (**1** glyme as ligand, polymerization at 20°C. 126 MHz, chloroform-d).

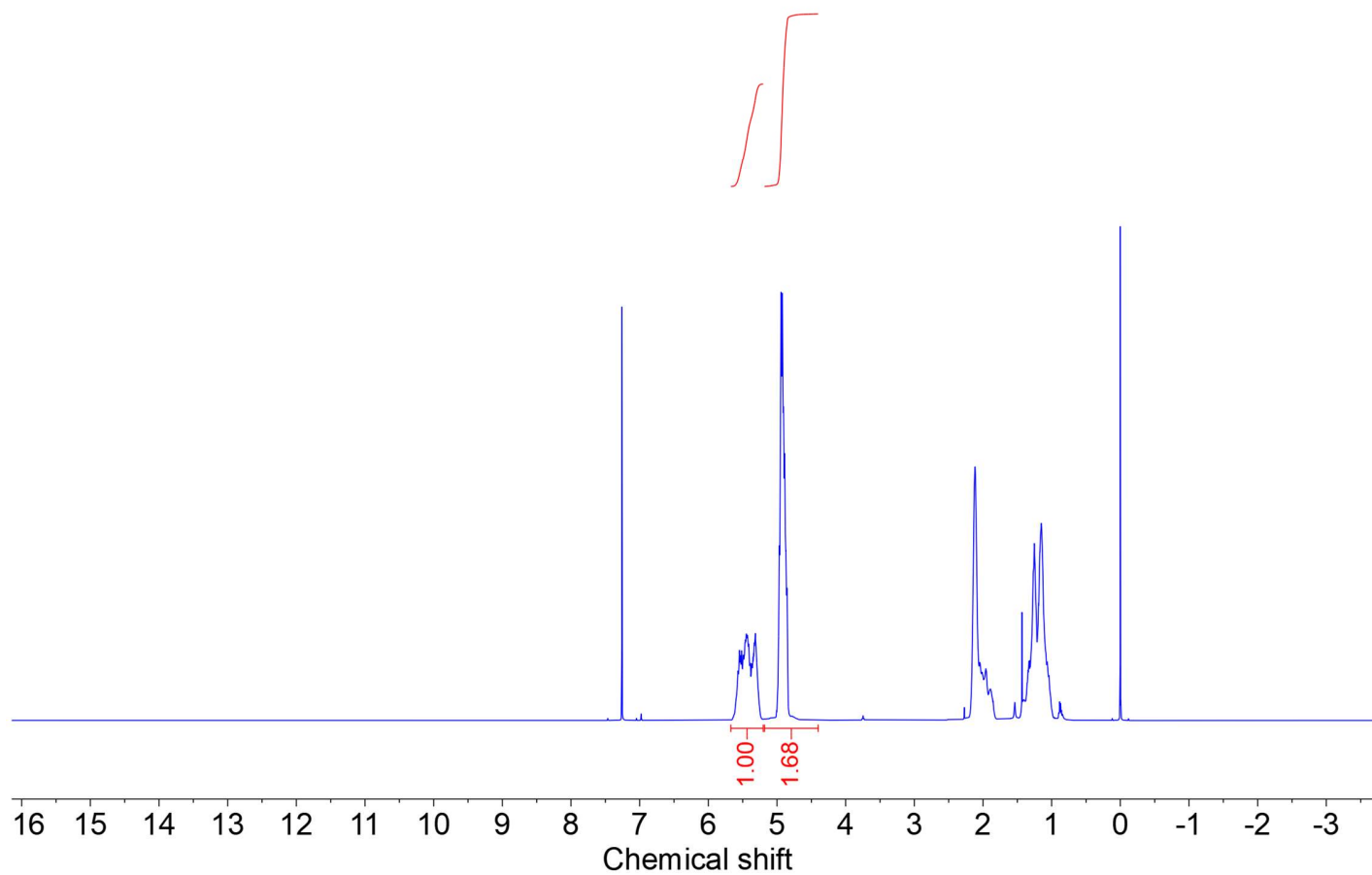


Figure S77. ^1H NMR spectrum of polybutadiene in entry 2 of Table 1 (**2** THF as ligand, polymerization at 20°C. 500 MHz, chloroform-d).

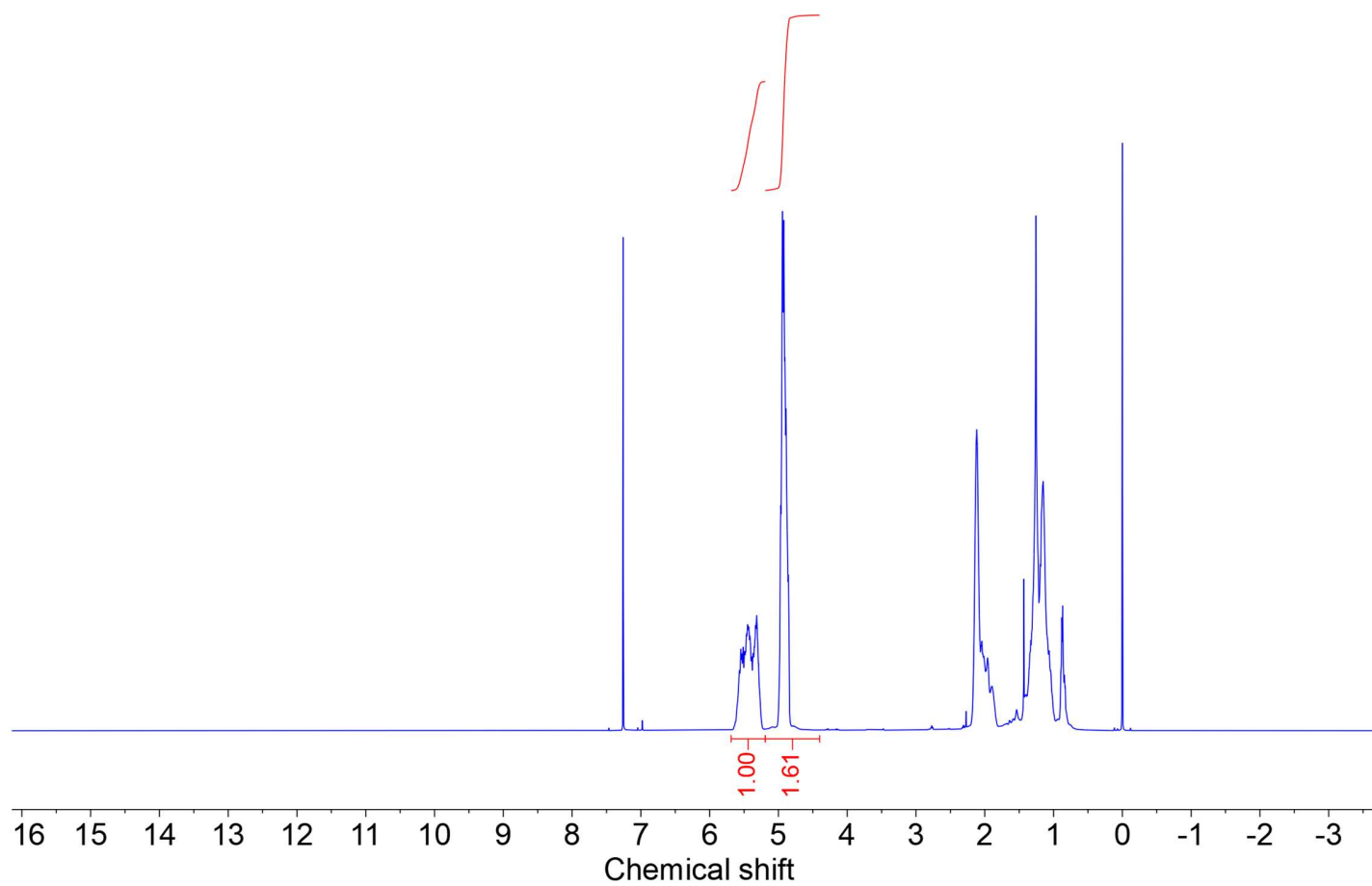


Figure S78. ^1H NMR spectrum of polybutadiene (**2** THF as ligand, polymerization at 0°C . 500 MHz, chloroform- d).

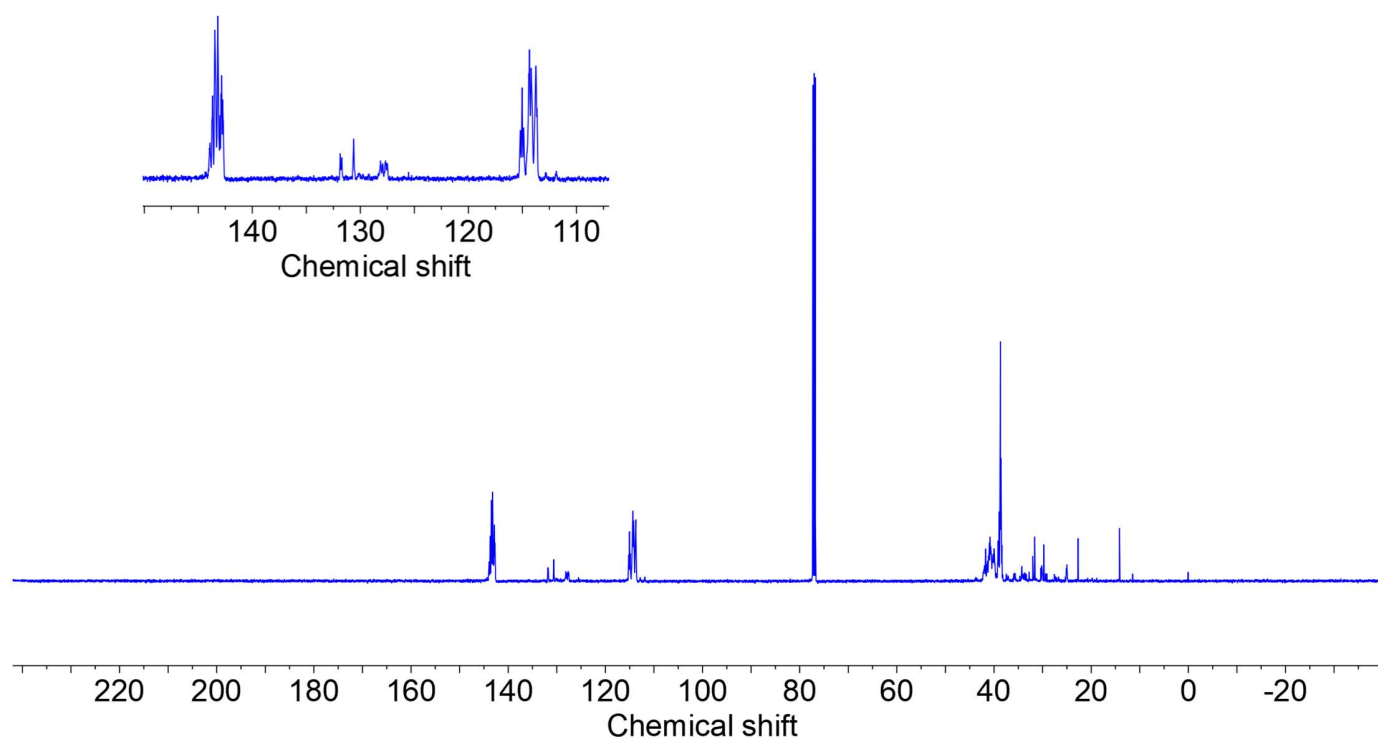


Figure S79. ^{13}C NMR spectrum of polybutadiene in entry 2 of Table 1 (**2** THF as ligand, polymerization at 20°C. 126 MHz, chloroform-d).

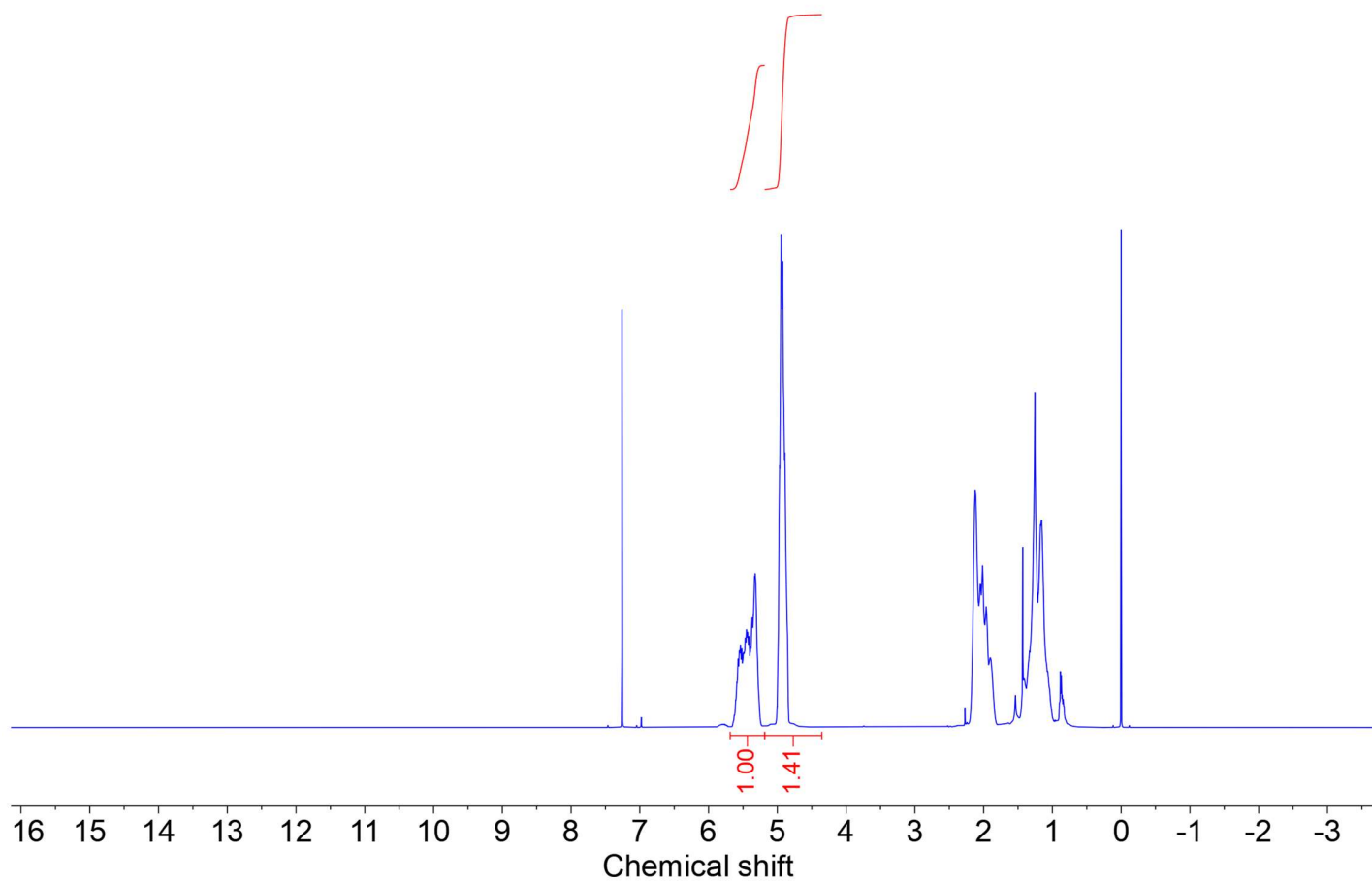


Figure S80. ^1H NMR spectrum of polybutadiene in entry 3 of Table 1 (**3** TMEDA as ligand, polymerization at 20°C. 500 MHz, chloroform-d).

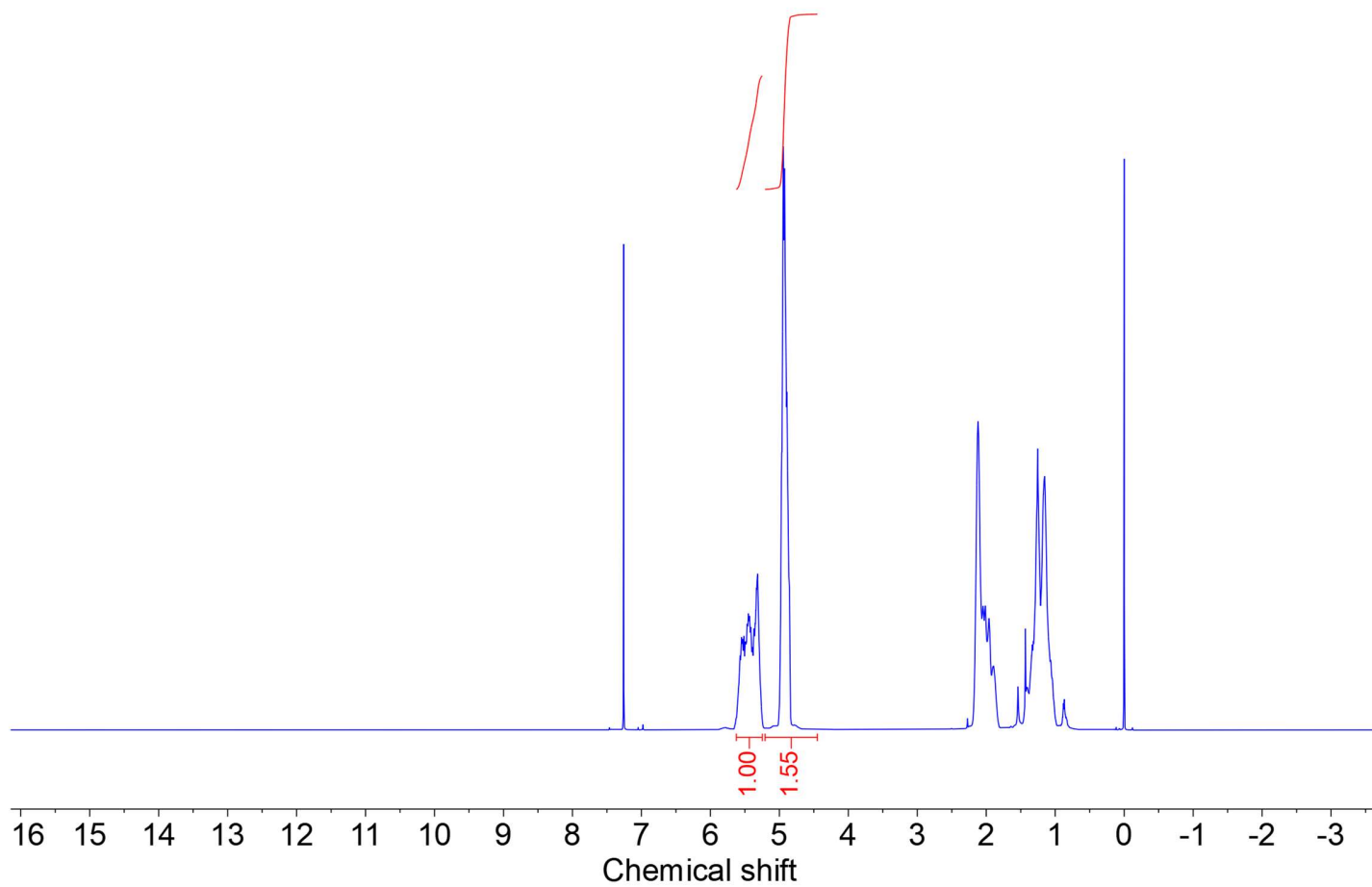


Figure S81. ^1H NMR spectrum of polybutadiene (**3** TMEDA as ligand, polymerization at 0°C . 500 MHz, chloroform- d).

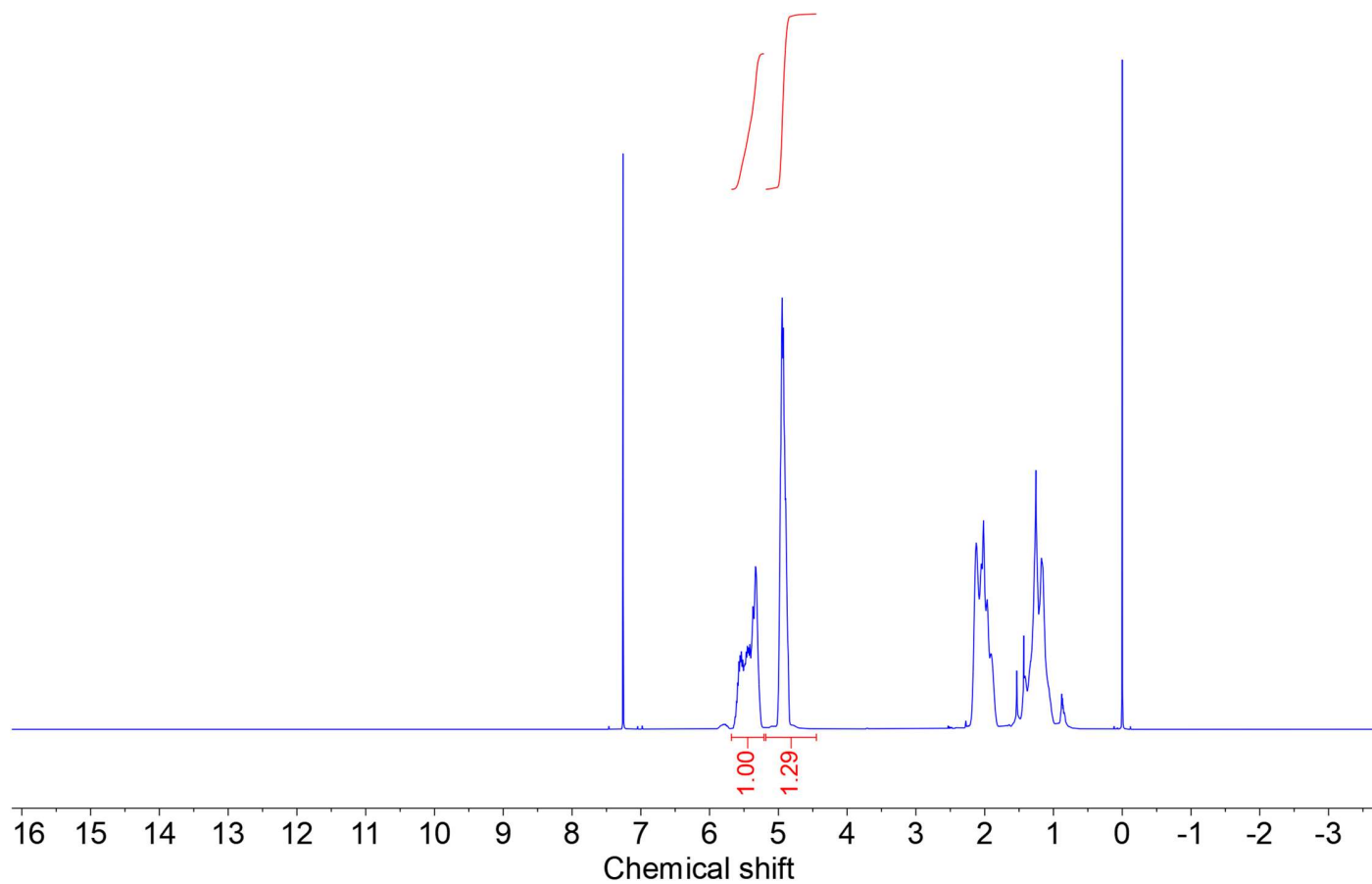


Figure S82. ^1H NMR spectrum of polybutadiene (**3** TMEDA as ligand, polymerization at 40°C. 500 MHz, chloroform-d).

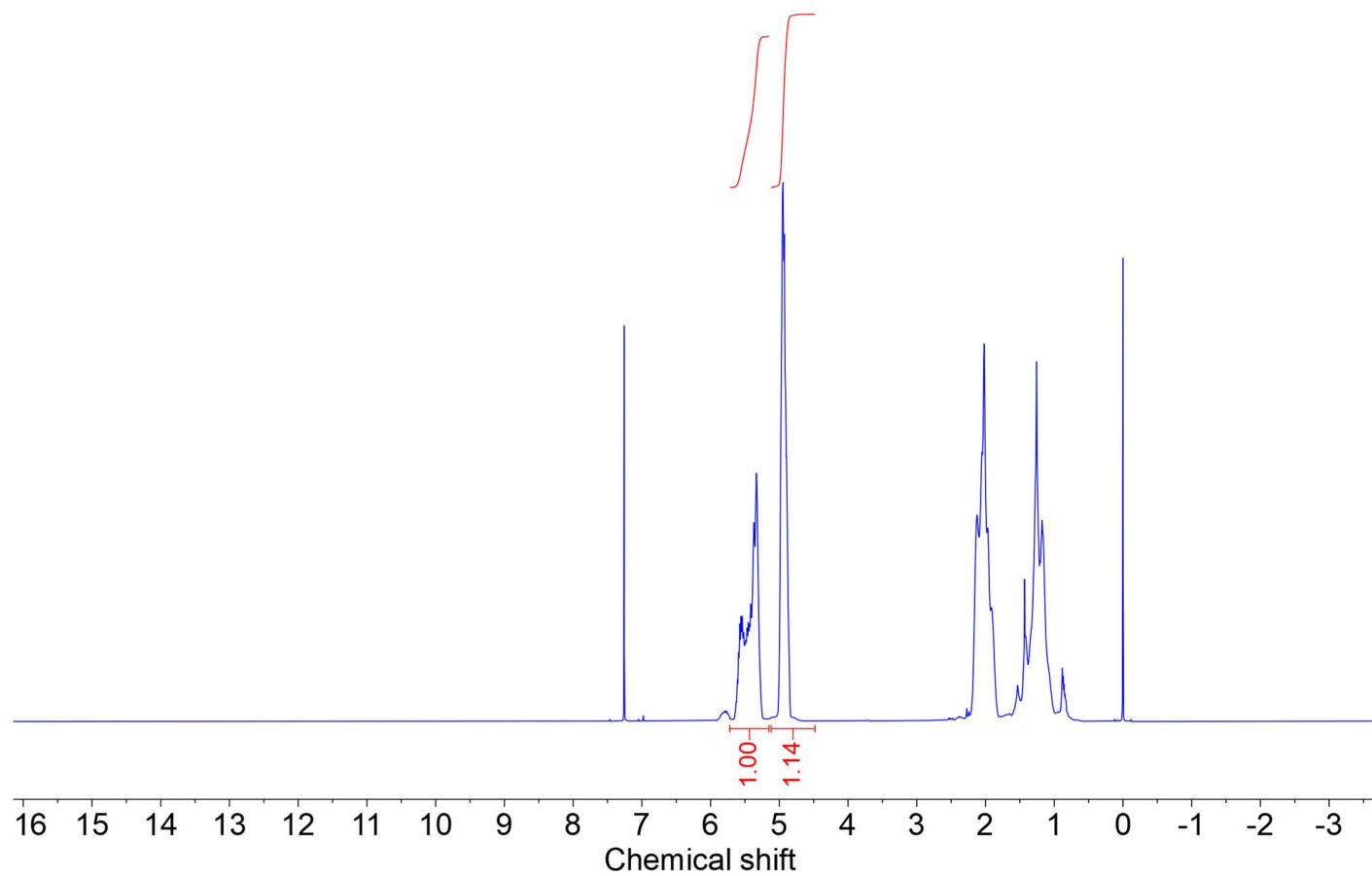


Figure S83. ^1H NMR spectrum of polybutadiene (**3** TMEDA as ligand, polymerization at 60°C. 500 MHz, chloroform-d).

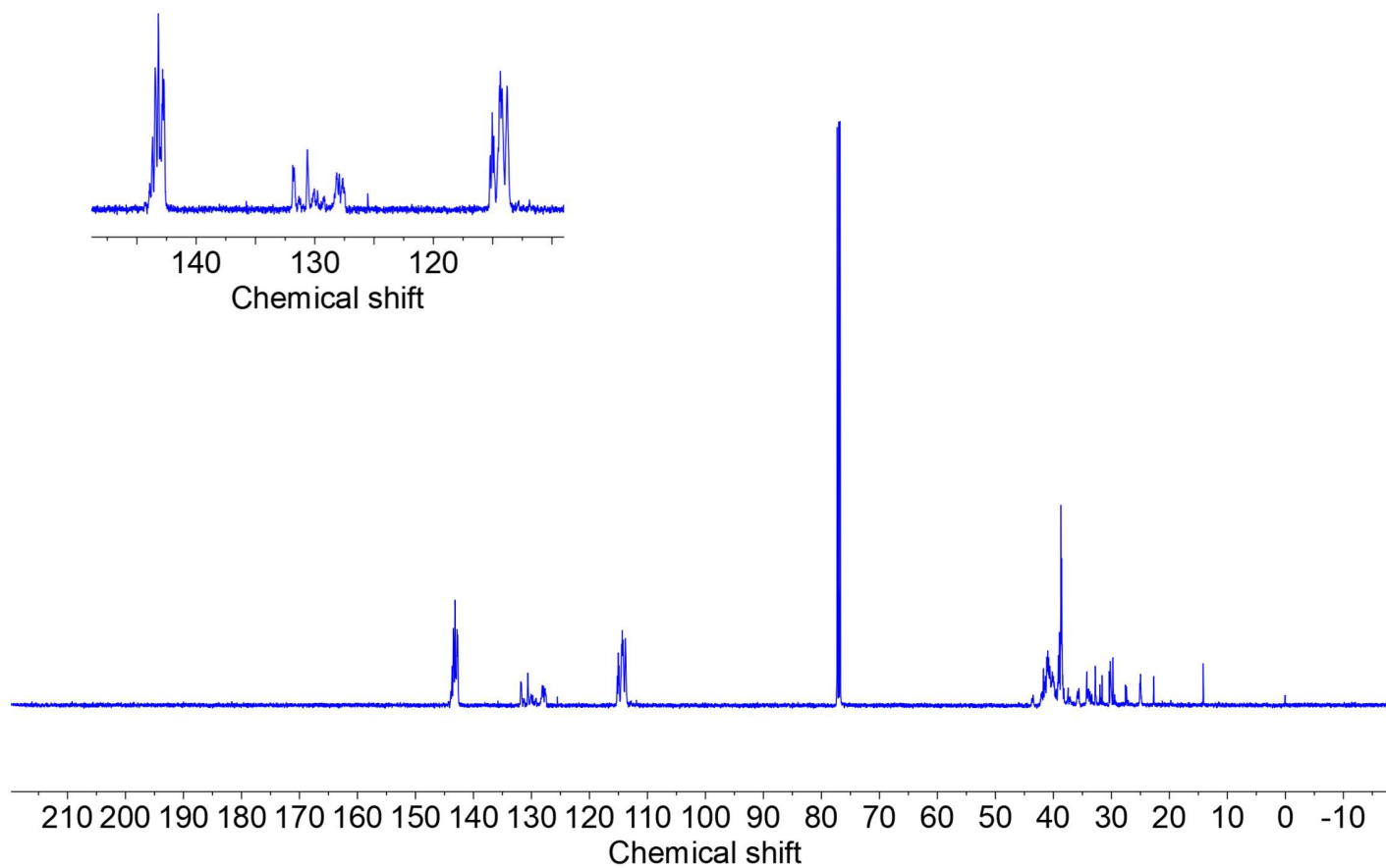


Figure S84. ^{13}C NMR spectrum of polybutadiene in entry 3 of Table 1 (**3** TMEDA as ligand, polymerization at 20°C. 126 MHz, chloroform-d).

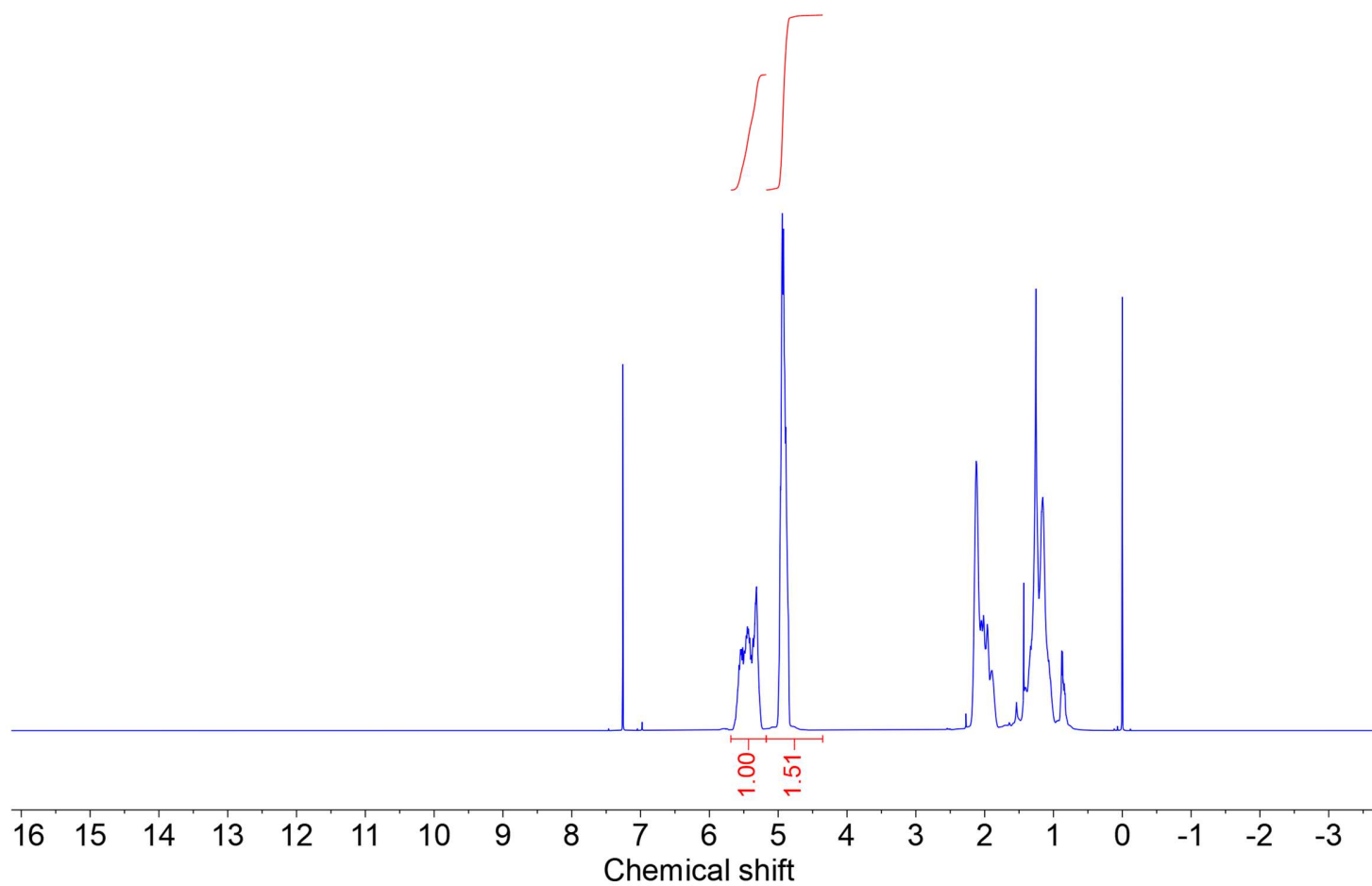


Figure S85. ^1H NMR spectrum of polybutadiene in entry 4 of Table 1 (**4** TEEDA as ligand, polymerization at 20°C. 500 MHz, chloroform-d).

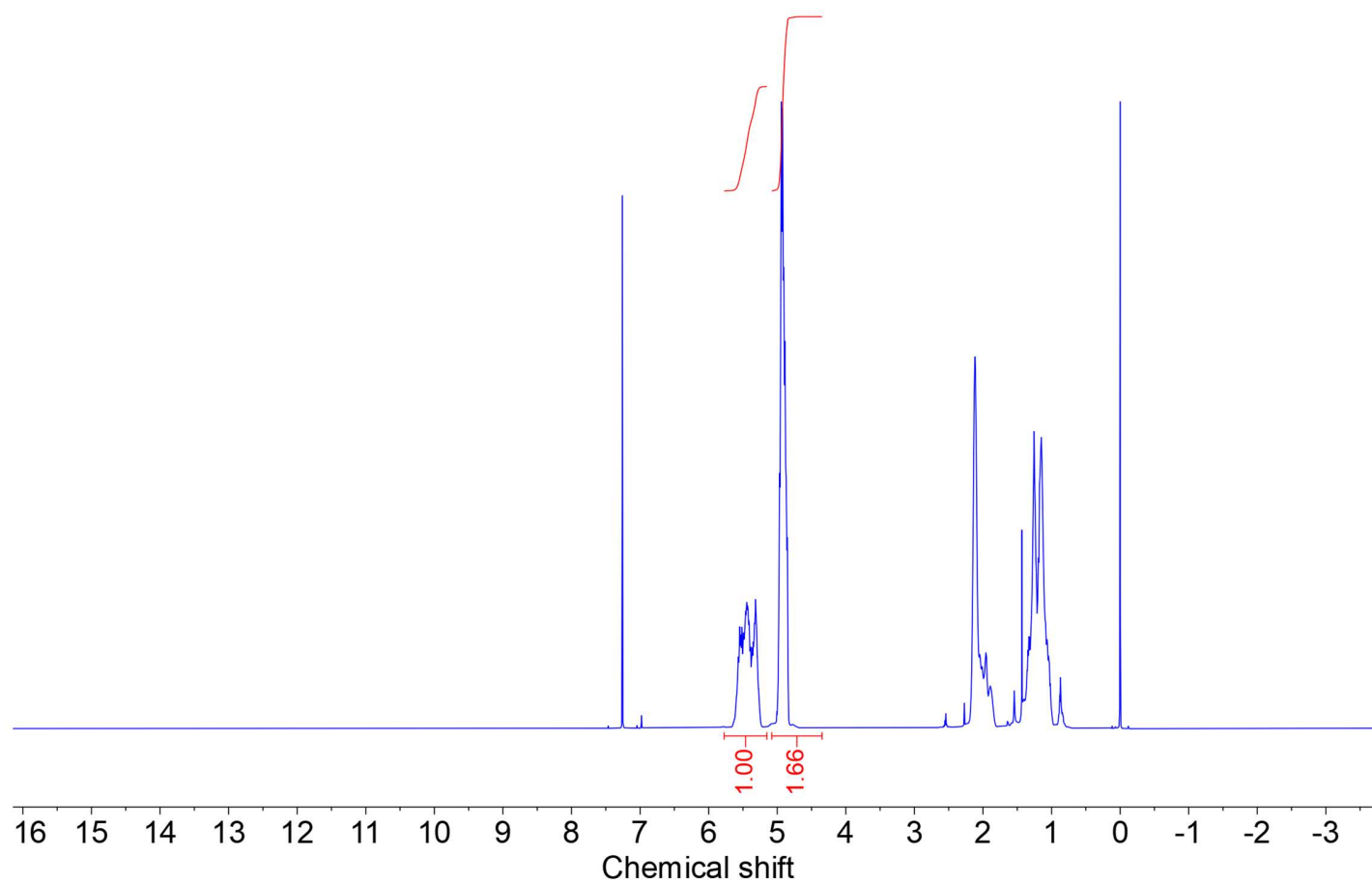


Figure S86. ^1H NMR spectrum of polybutadiene (4 TEEDA as ligand, polymerization at 0°C . 500 MHz, chloroform-d).

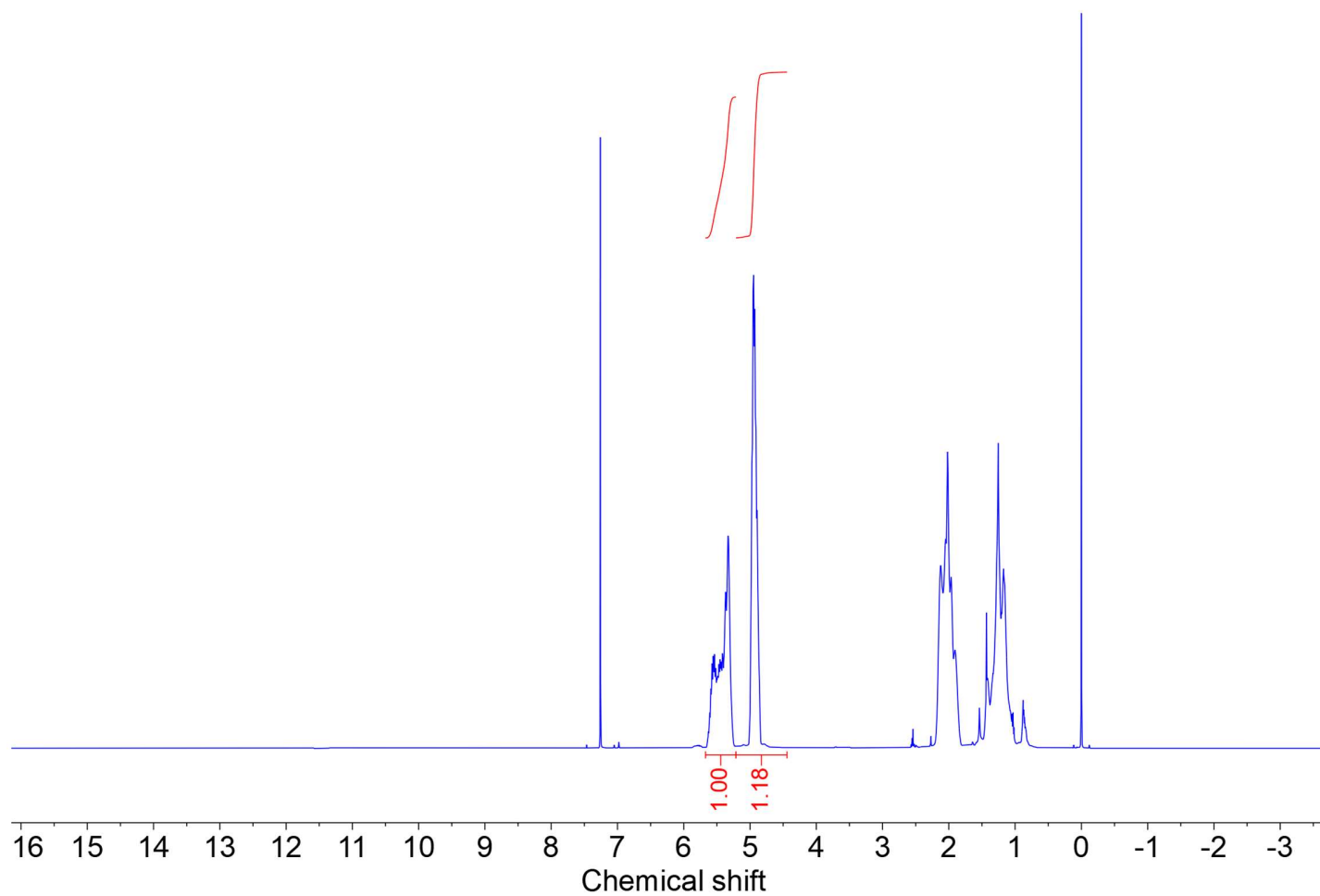


Figure S87. ^1H NMR spectrum of polybutadiene (**4** TEEDA as ligand, polymerization at 40°C. 500 MHz, chloroform-d).

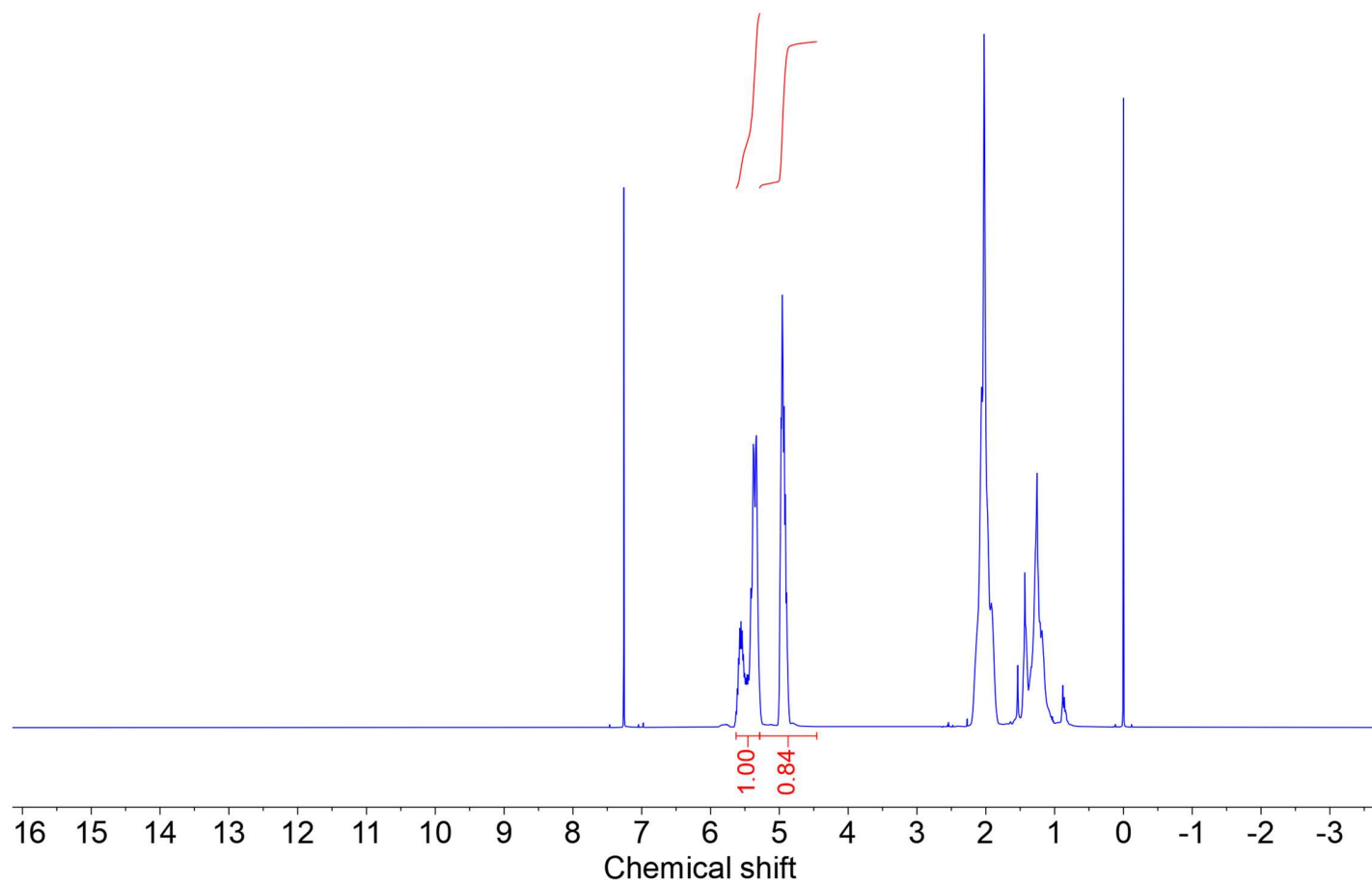


Figure S88. ^1H NMR spectrum of polybutadiene (**4** TEEDA as ligand, polymerization at 60°C. 500 MHz, chloroform-d).

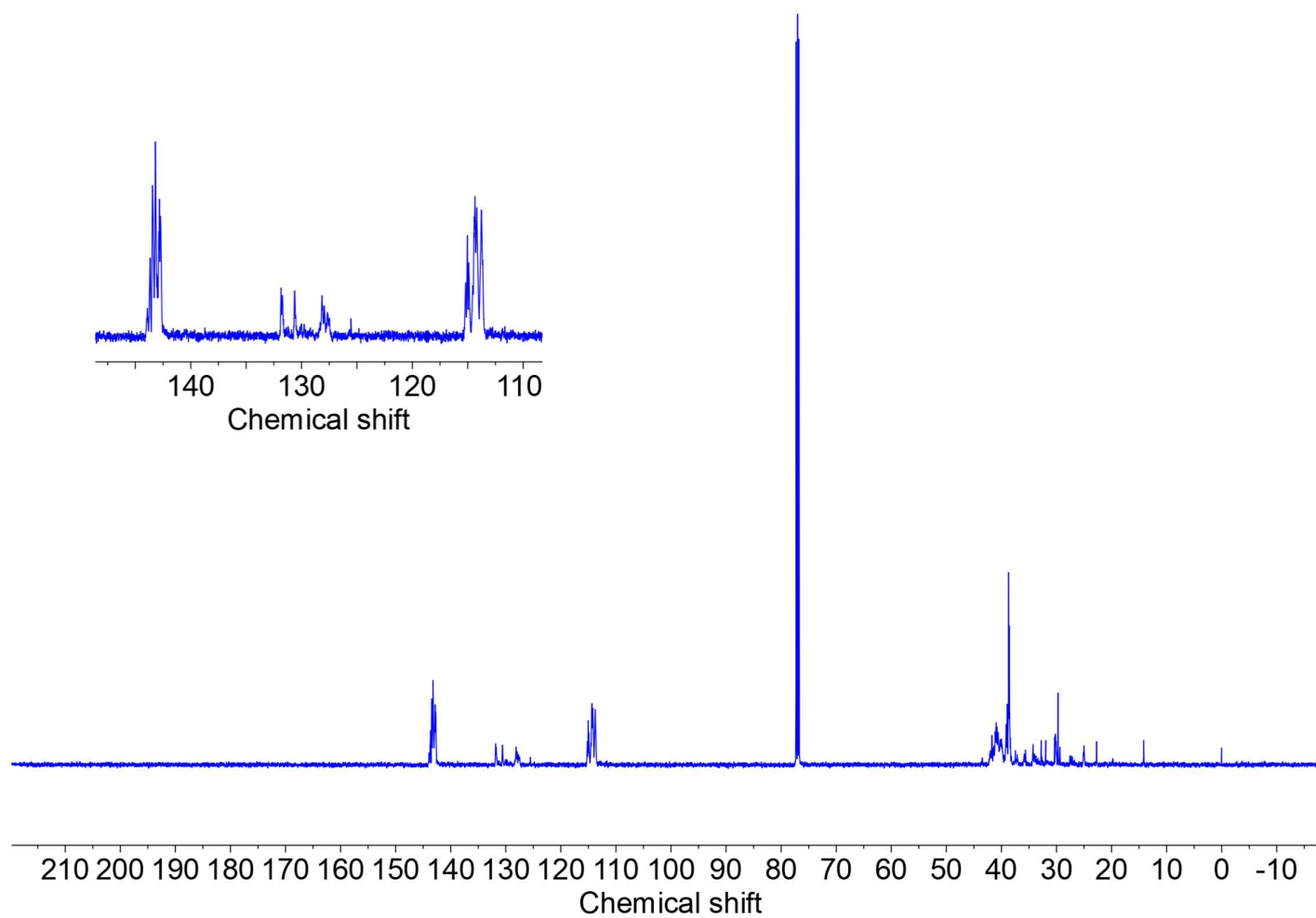


Figure S89. ^{13}C NMR spectrum of polybutadiene in entry 4 of Table 1 (**4** TEEDA as ligand, polymerization at 20°C. 500 MHz, chloroform-d).

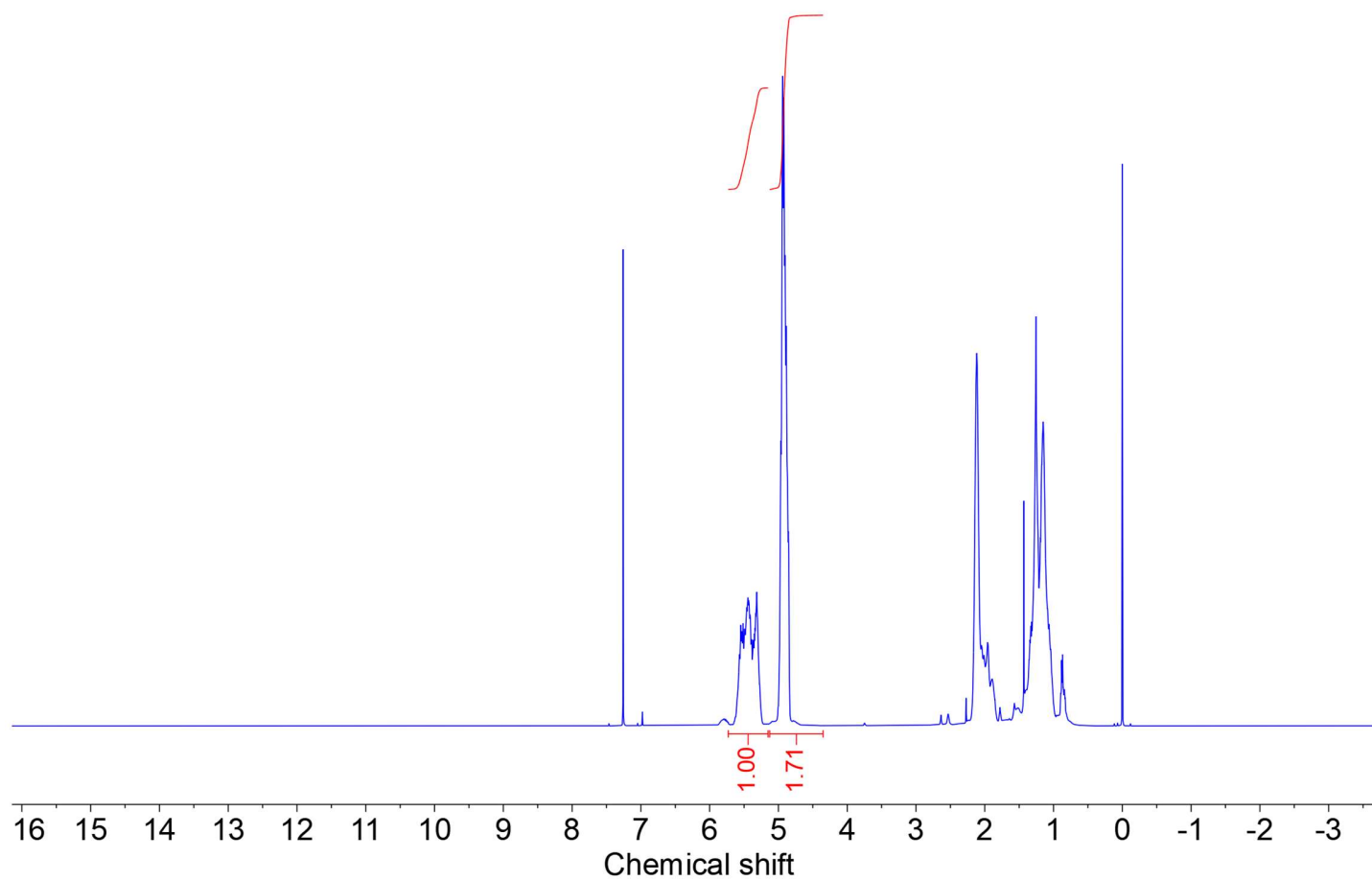


Figure S90. ^1H NMR spectrum of polybutadiene in entry 5 of Table 1 (**5** DiPyr as ligand, polymerization at 20°C. 500 MHz, chloroform-d).

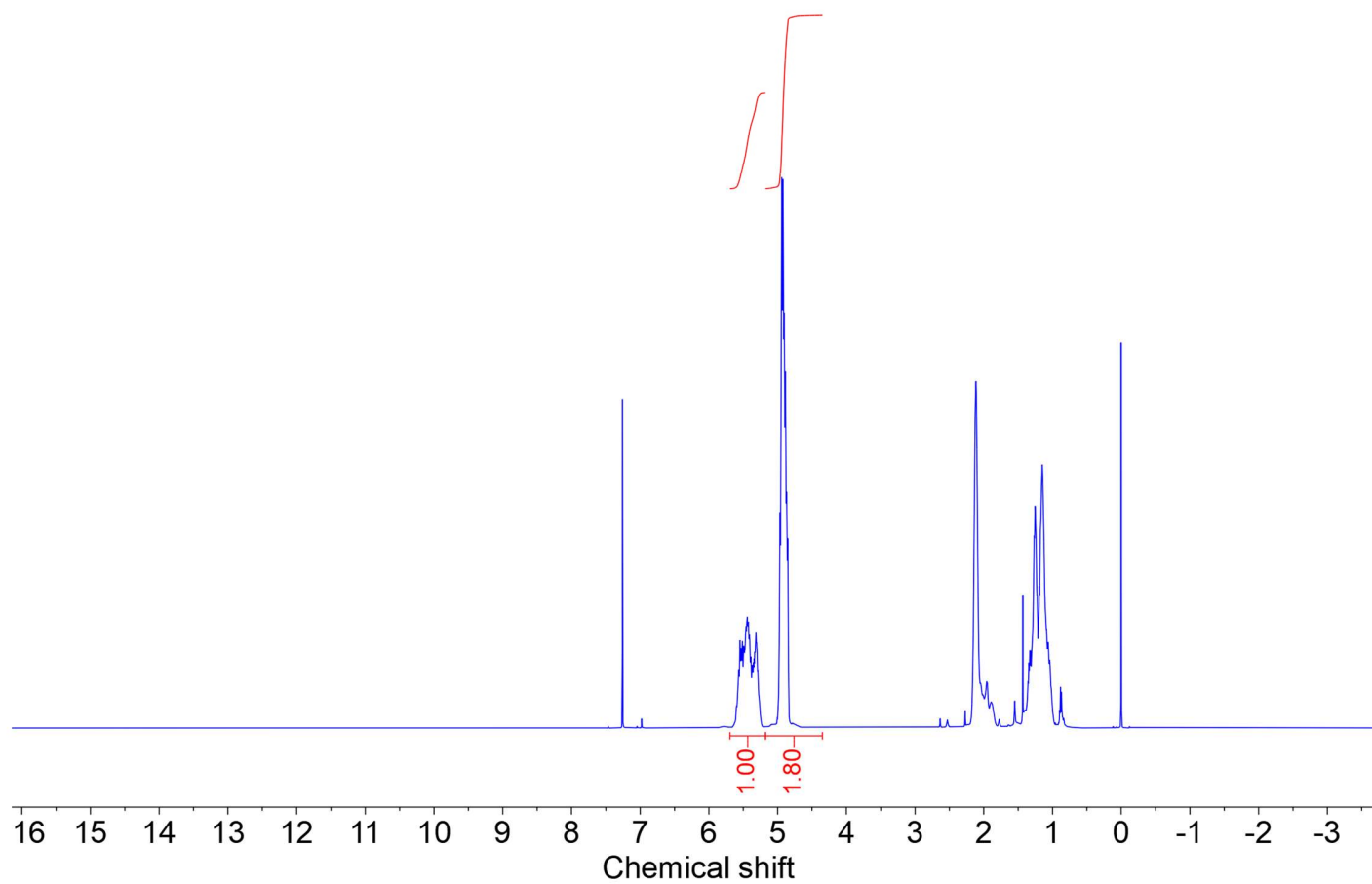


Figure S91. ^1H NMR spectrum of polybutadiene (5 DiPyr as ligand as ligand, polymerization at 0°C . 500 MHz, chloroform-d).

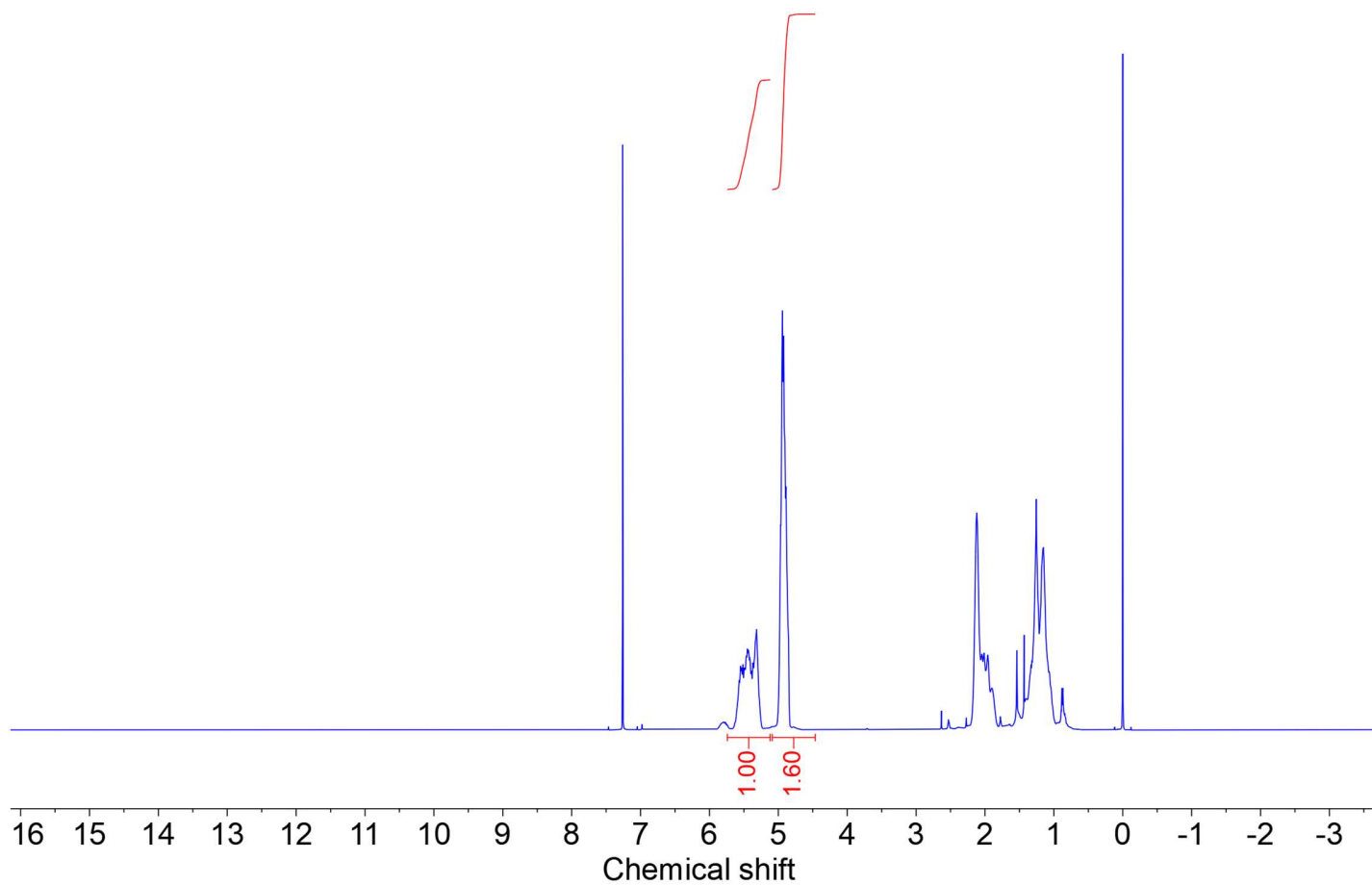


Figure S92. ^1H NMR spectrum of polybutadiene (5 DiPyr as ligand, polymerization at 40°C. 500 MHz, chloroform-d).

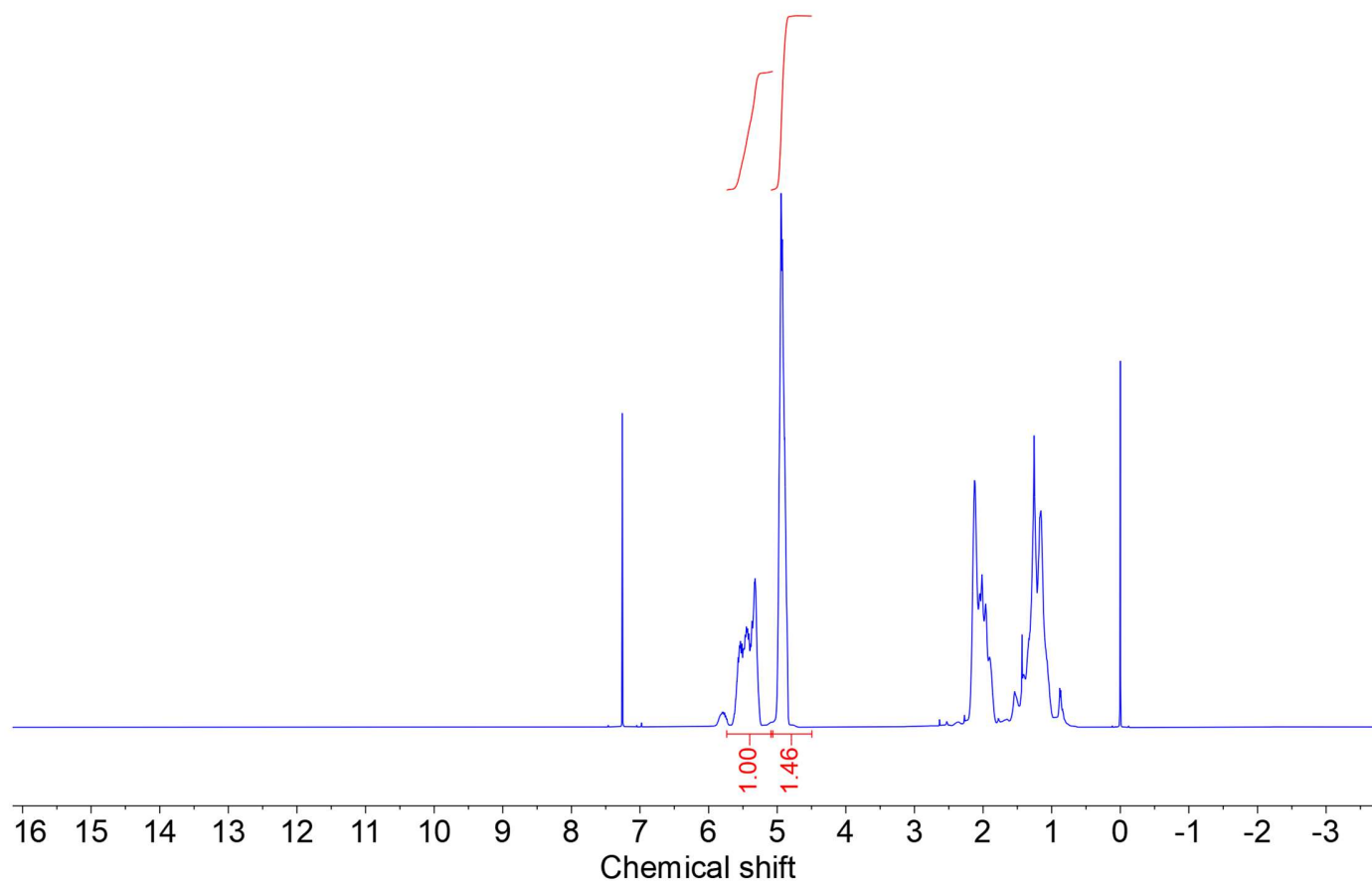


Figure S93. ^1H NMR spectrum of polybutadiene (**5** DiPyr as ligand, polymerization at 60°C. 500 MHz, chloroform-d).

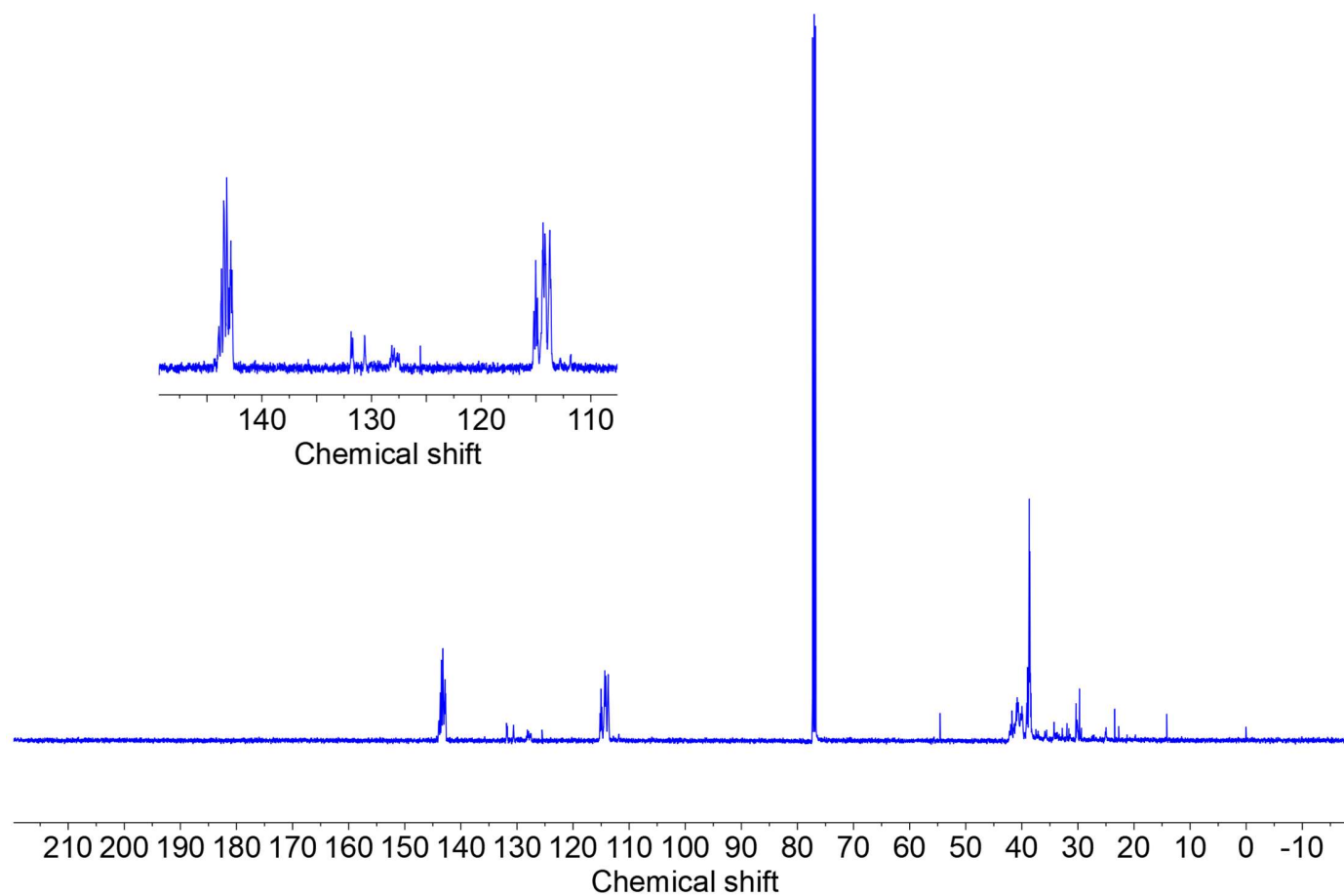


Figure S94. ^{13}C NMR spectrum of polybutadiene in entry 5 of Table 1 (5 DiPyr as ligand, polymerization at 20°C. 126 MHz, chloroform-d).

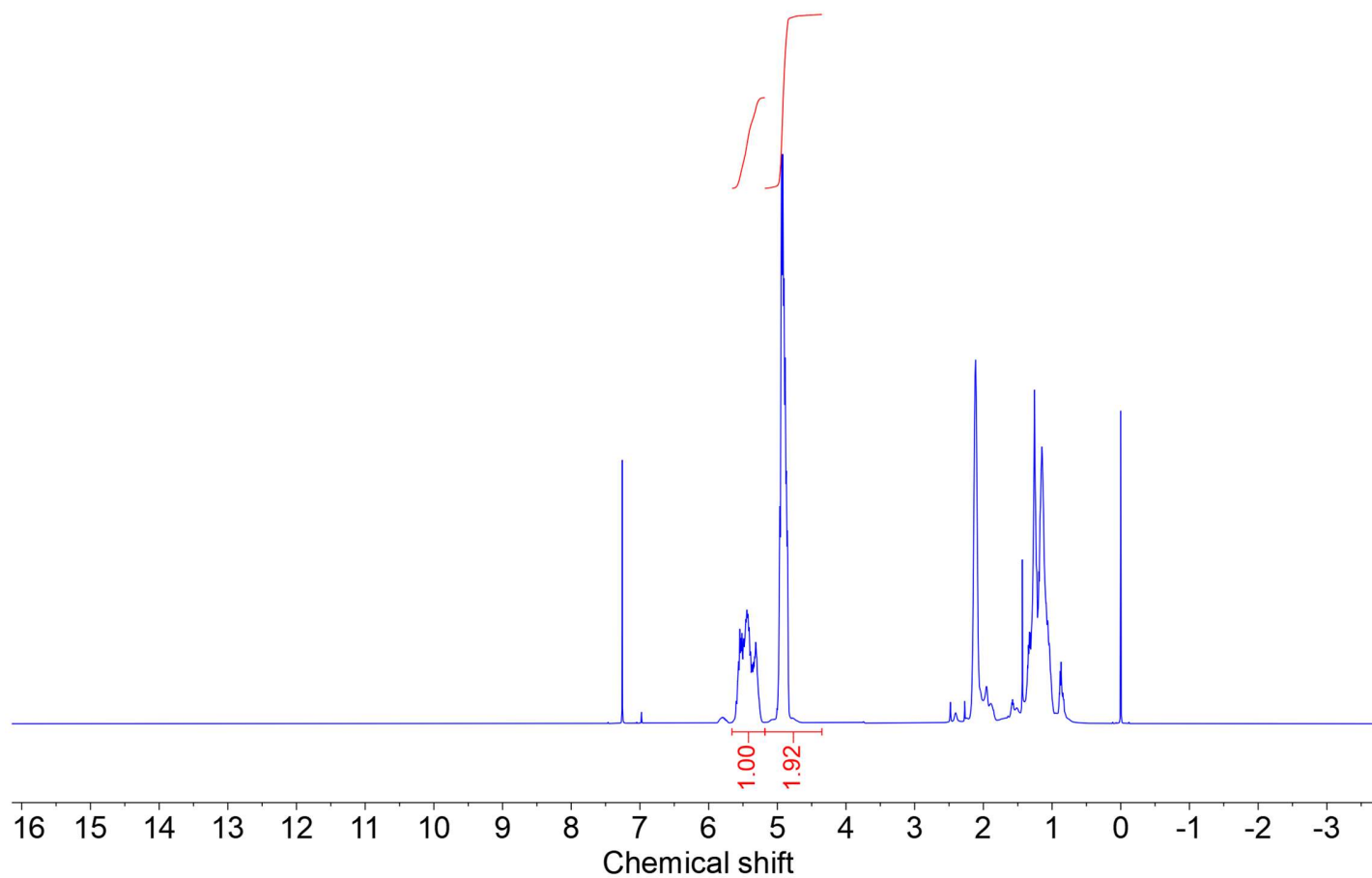


Figure S95. ^1H NMR spectrum of polybutadiene in entry 6 of Table 1 (**6** DiPip as ligand, polymerization at 20°C. 500 MHz, chloroform-d).

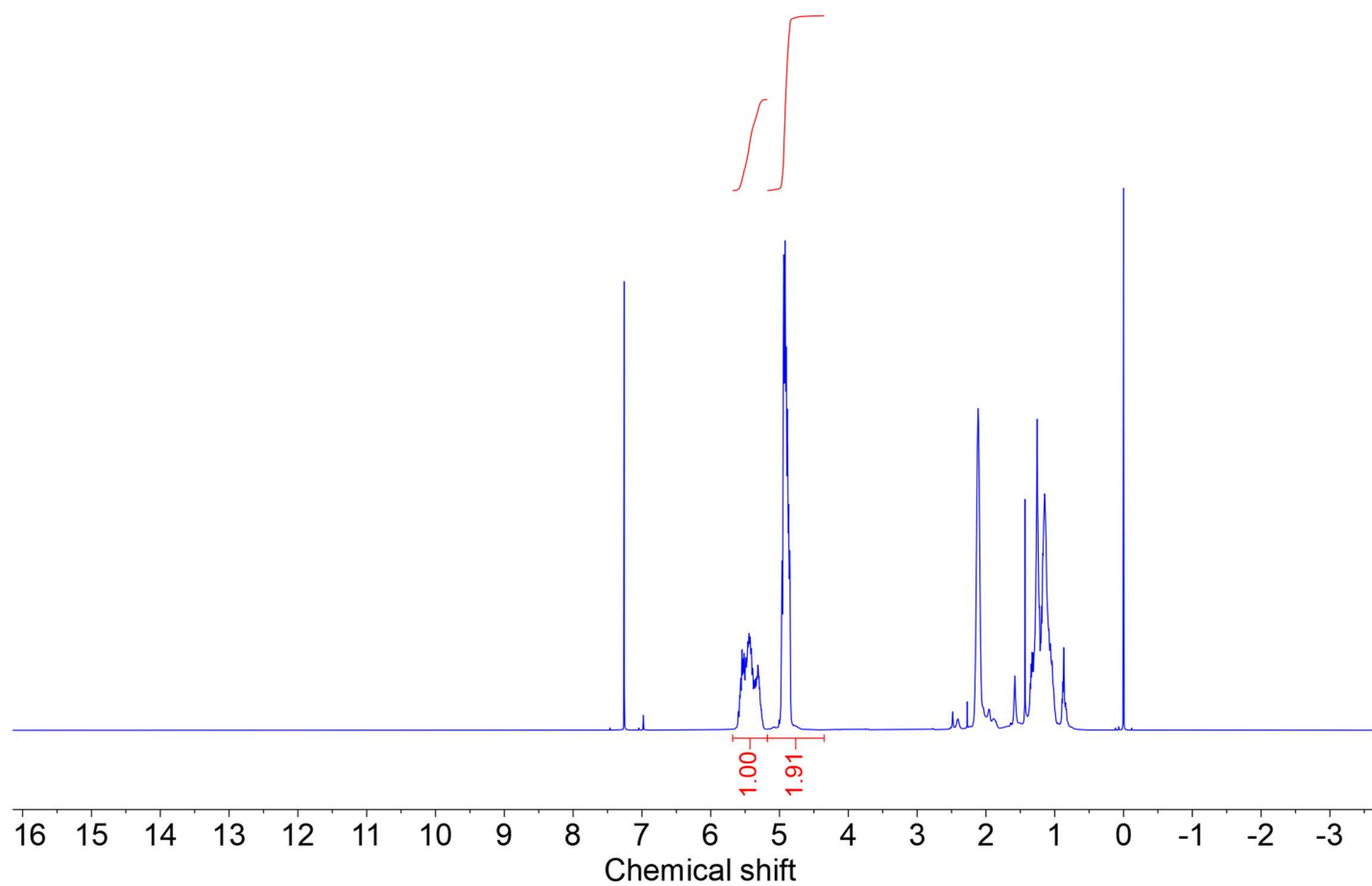


Figure S96. ^1H NMR spectrum of polybutadiene (6 DiPip as ligand, polymerization at 0°C . 500 MHz, chloroform-d).

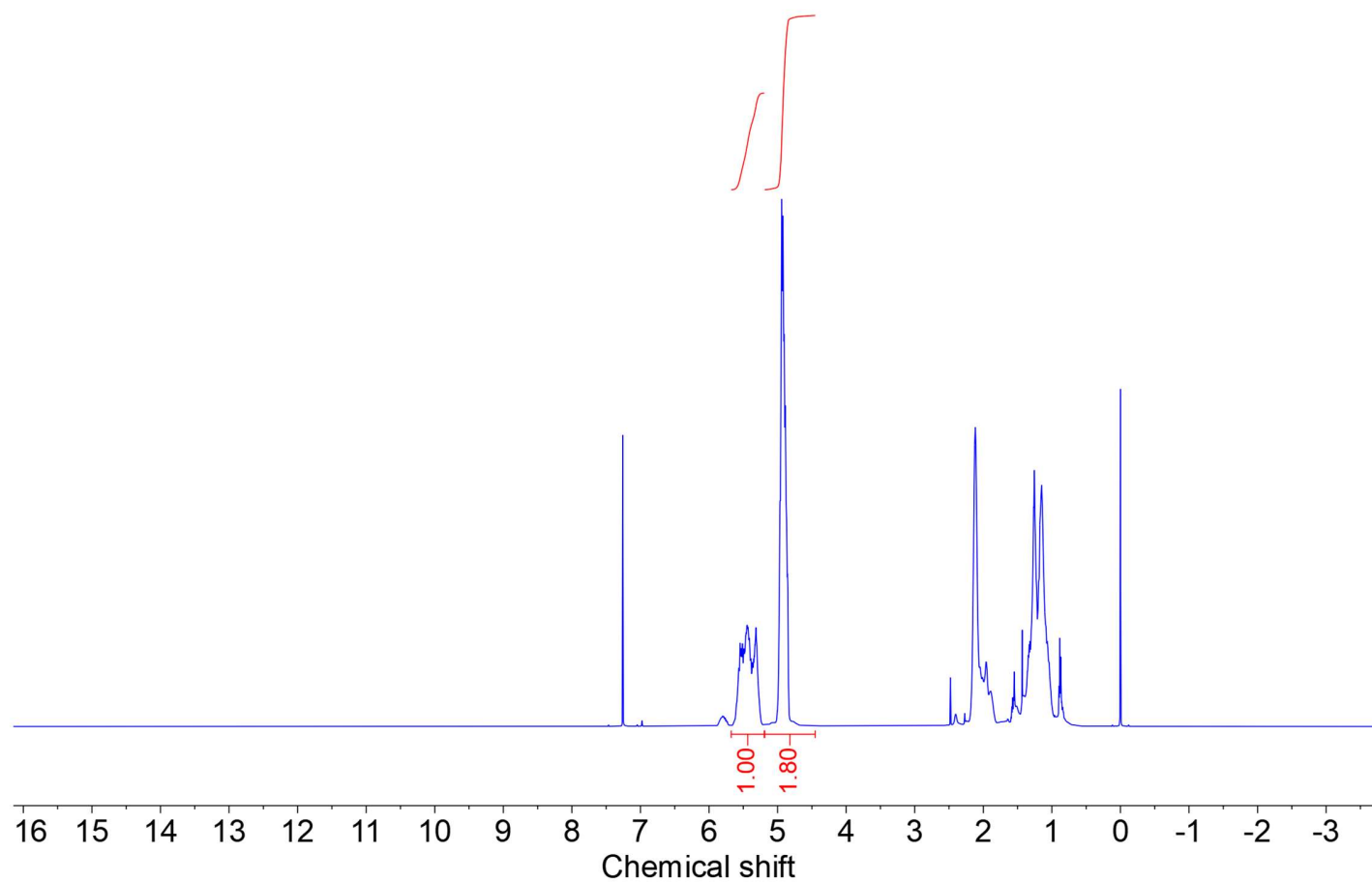


Figure S97. ^1H NMR spectrum of polybutadiene (**6** DiPip as ligand, polymerization at 40°C. 500 MHz, chloroform-d).

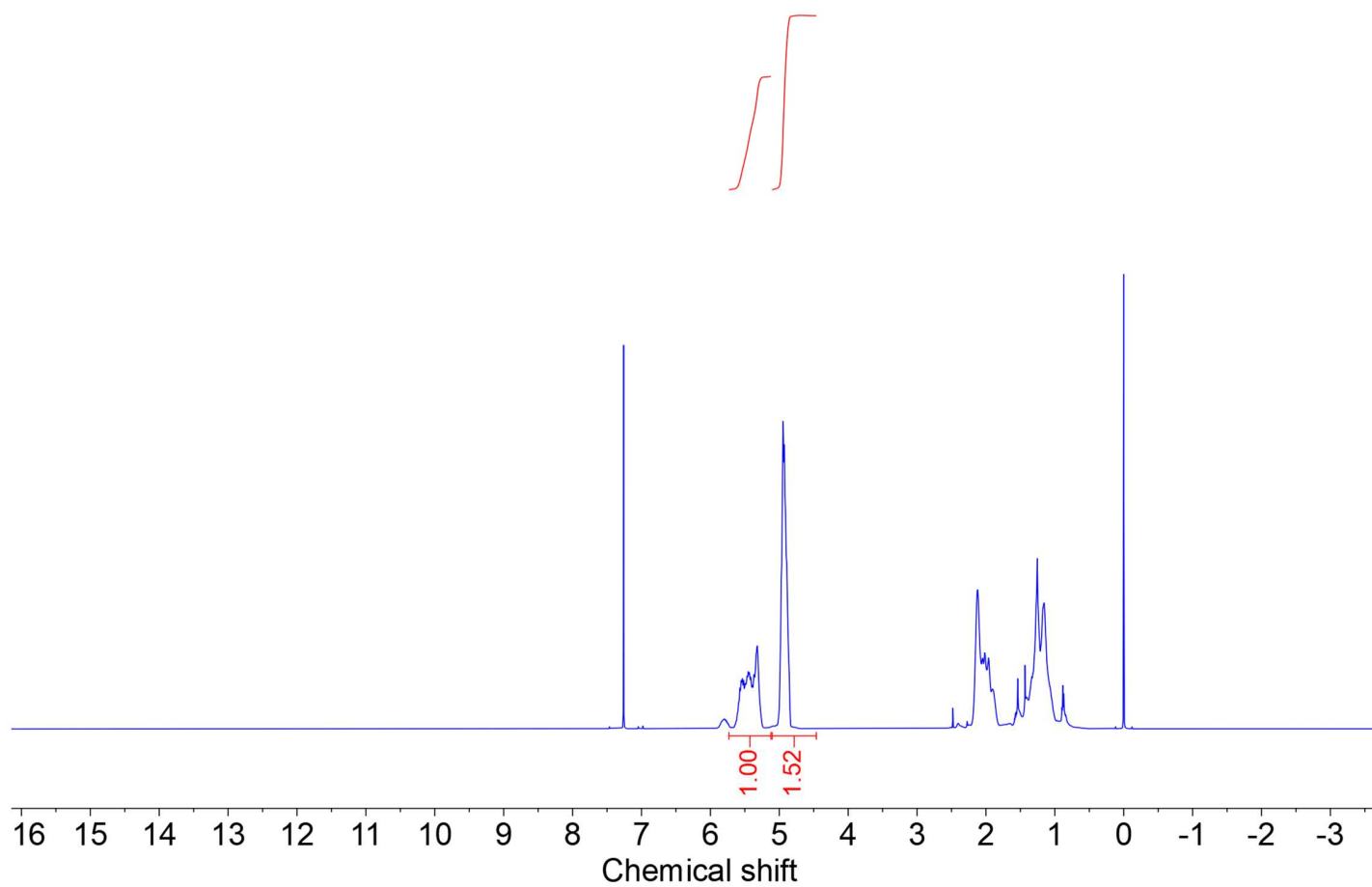


Figure S98. ^1H NMR spectrum of polybutadiene (**6** DiPip as ligand, polymerization at 60°C. 500 MHz, chloroform-d).

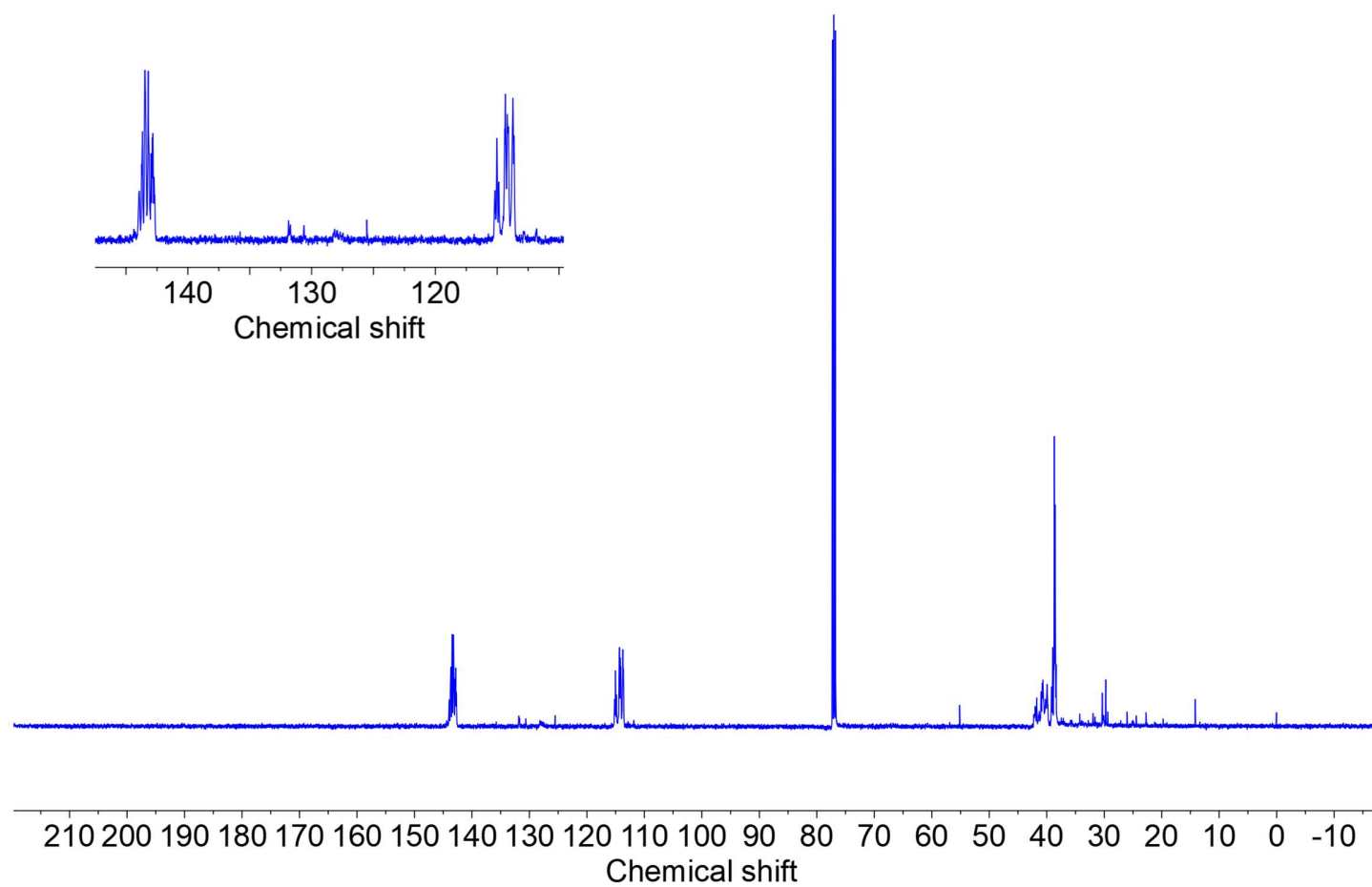


Figure S99. ^{13}C NMR spectrum of polybutadiene in entry 6 of Table 1 (**6** DiPip as ligand, polymerization at 20°C. 126 MHz, chloroform-d).

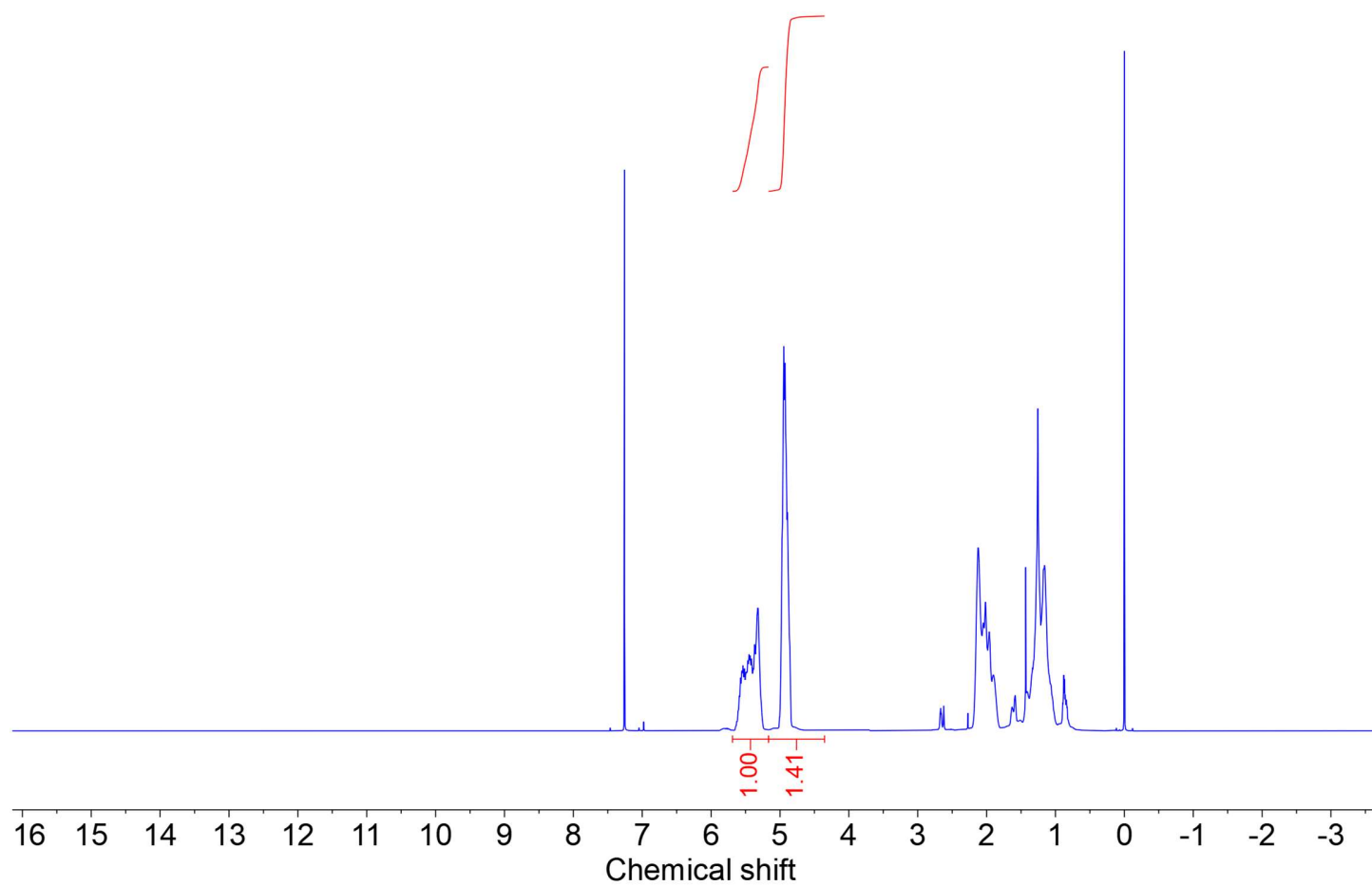


Figure S100. ^1H NMR spectrum of polybutadiene in entry 7 of Table 1 (**7** DiAze as ligand, polymerization at 20°C. 500 MHz, chloroform-d).

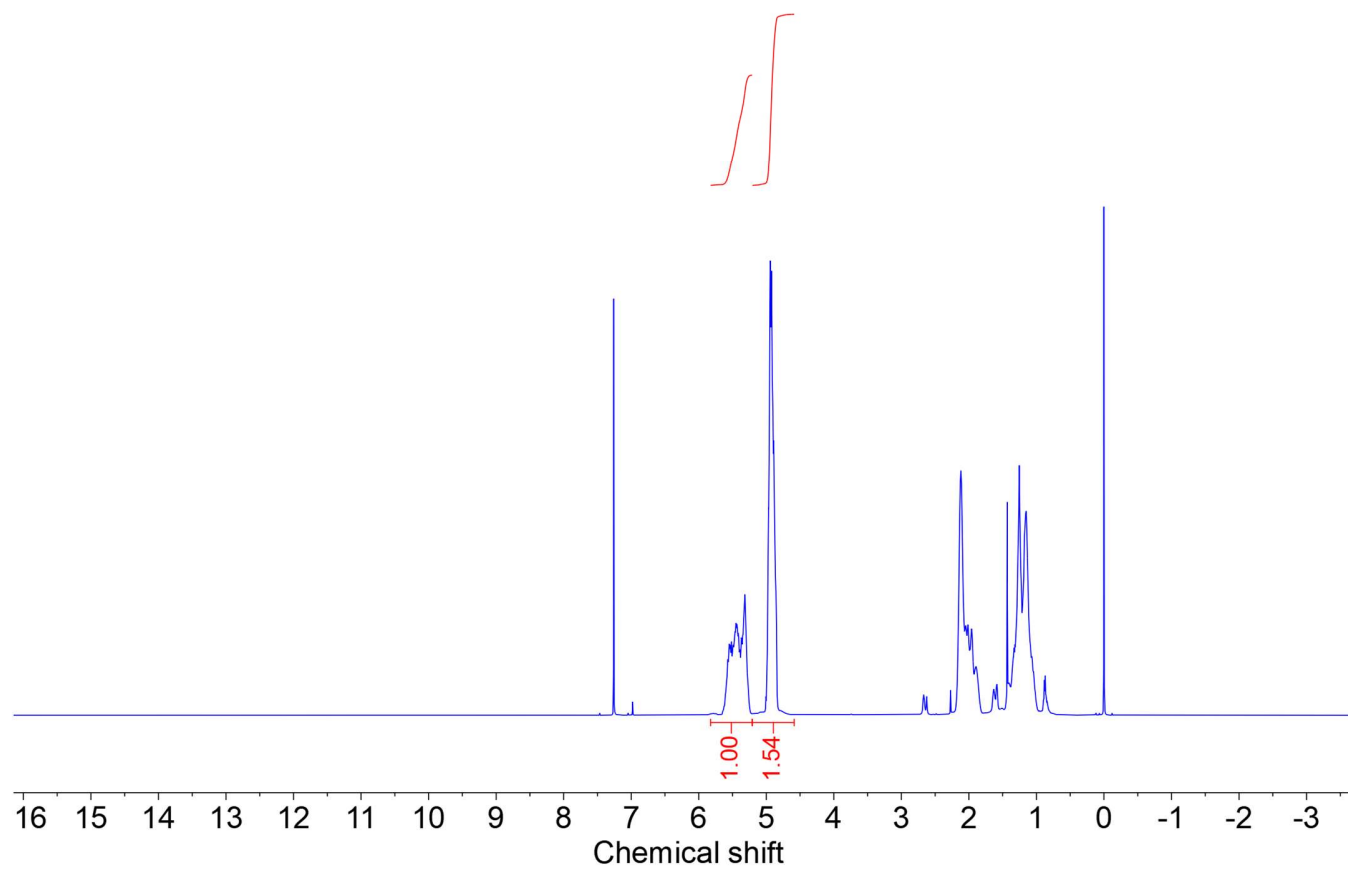


Figure S101. ^1H NMR spectrum of polybutadiene (7 DiAze as ligand, polymerization at 0°C . 500 MHz, chloroform-d).

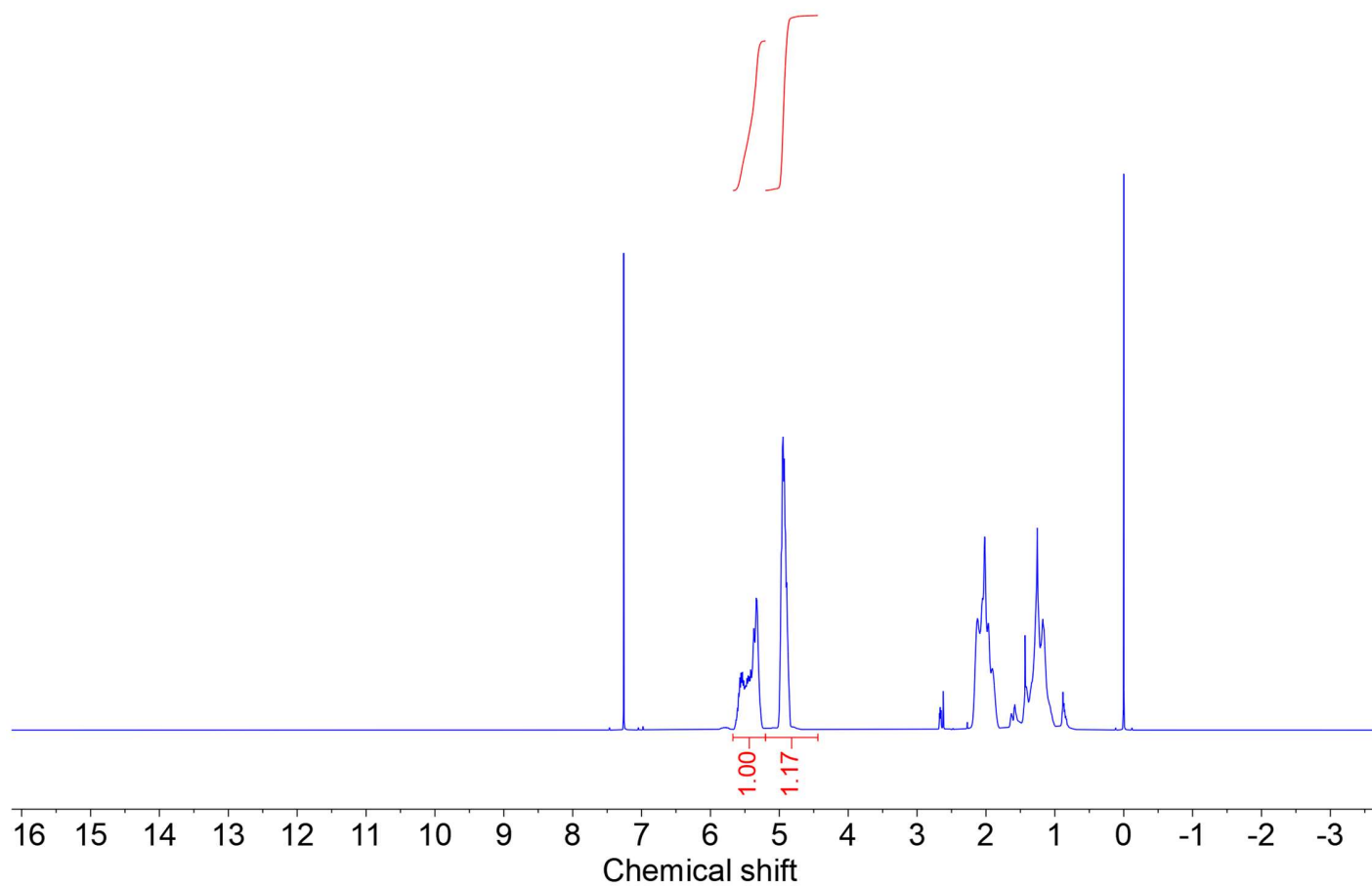


Figure S102. ^1H NMR spectrum of polybutadiene (**7** DiAze as ligand, polymerization at 40°C. 500 MHz, chloroform-d).

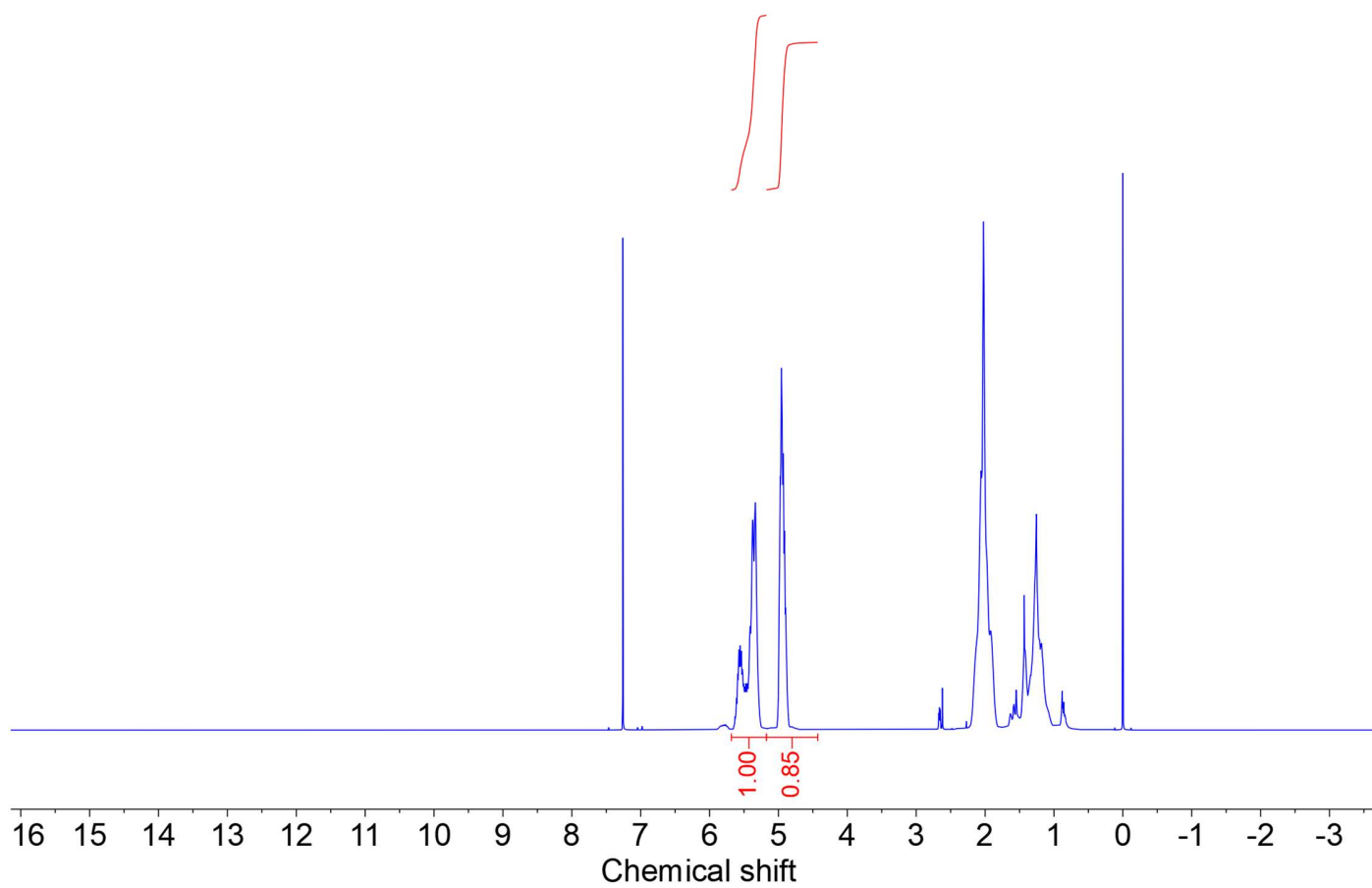


Figure S103. ^1H NMR spectrum of polybutadiene (**7** DiAze as ligand, polymerization at 60°C. 500 MHz, chloroform-d).

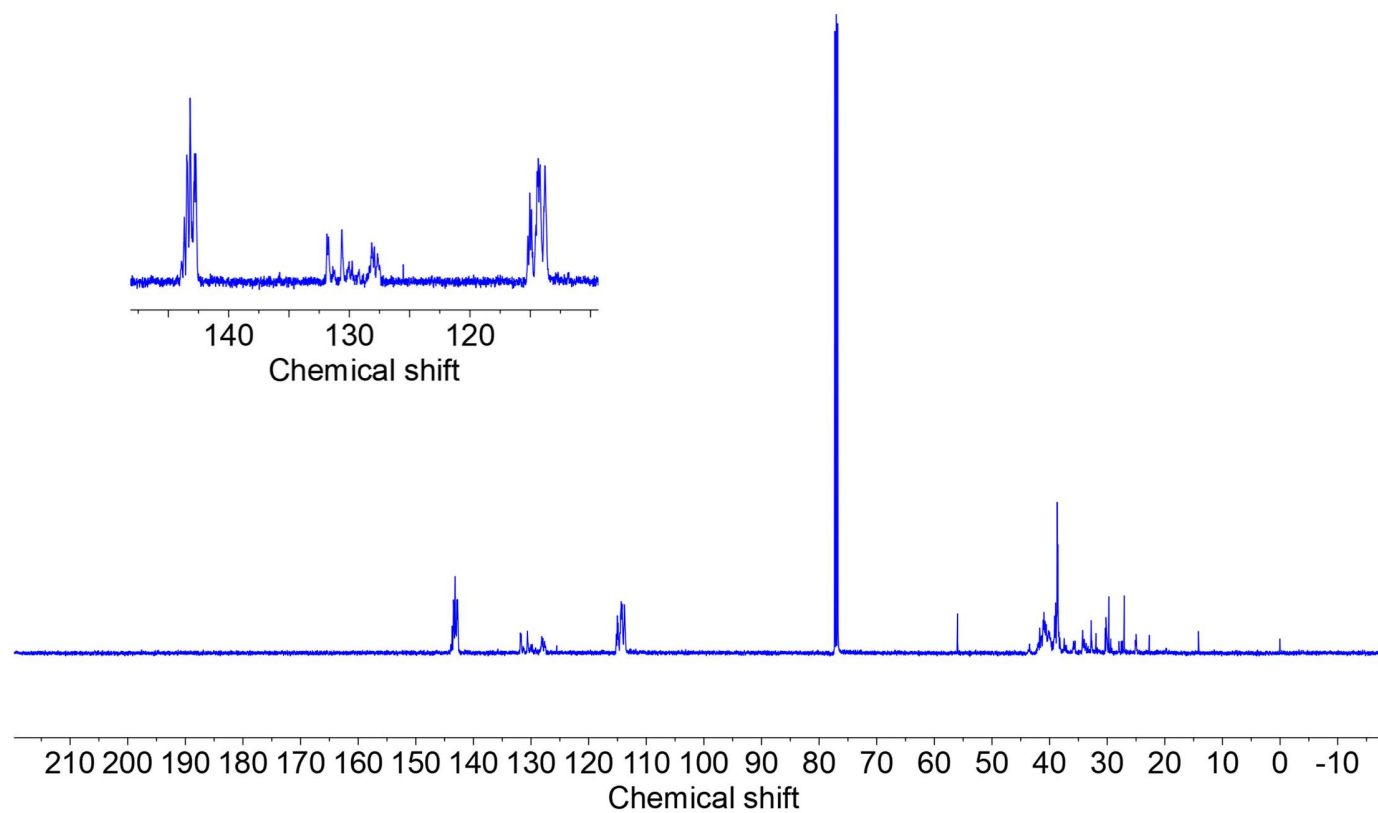


Figure S104. ^{13}C NMR spectrum of polybutadiene in entry 7 of Table 1 (**7** DiAze as ligand, polymerization at 20°C. 126 MHz, chloroform-d).

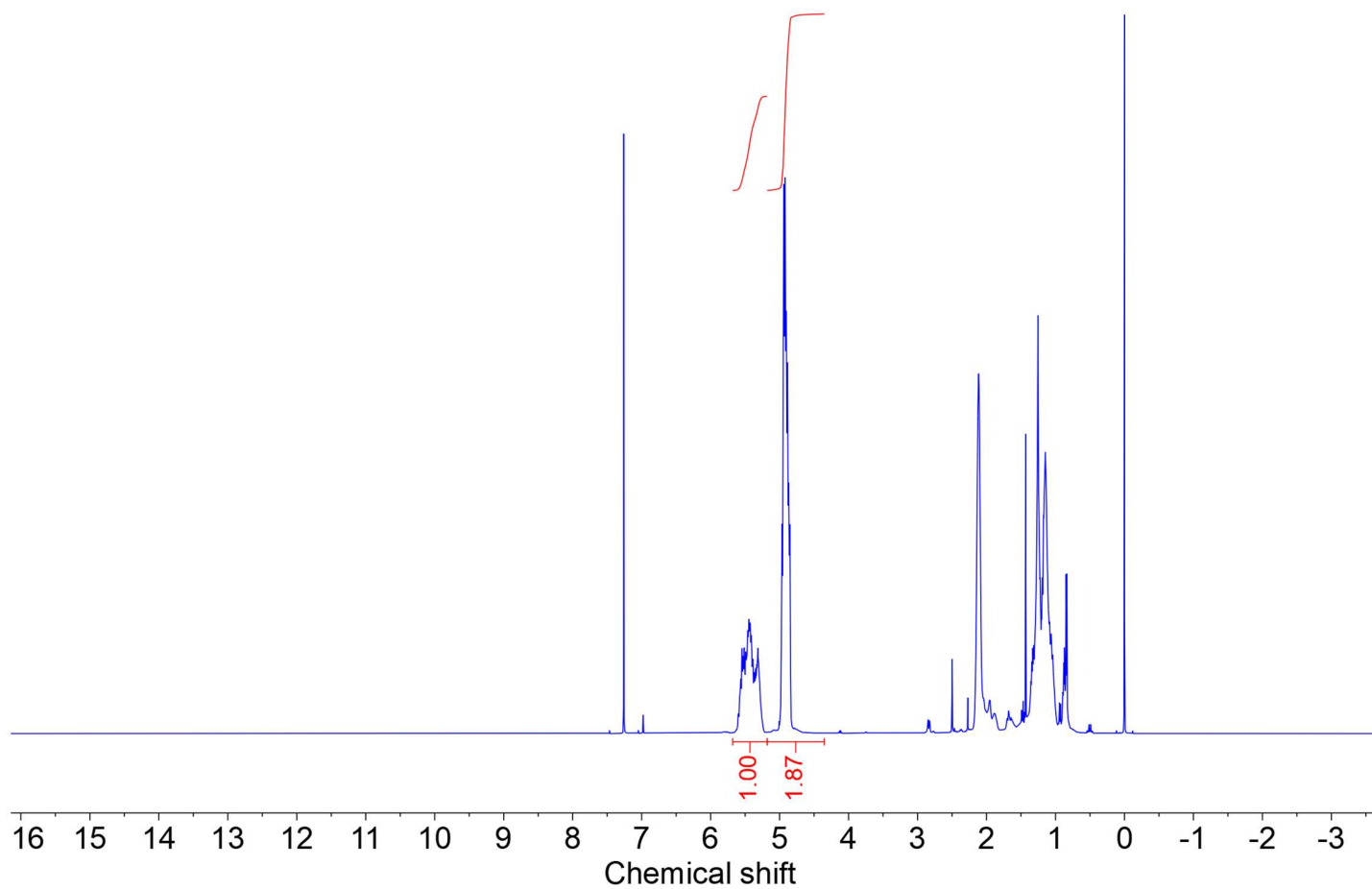


Figure S105. ^1H NMR spectrum of polybutadiene (**8** MeDiPip as ligand, polymerization at 20°C. 500 MHz, chloroform-d).

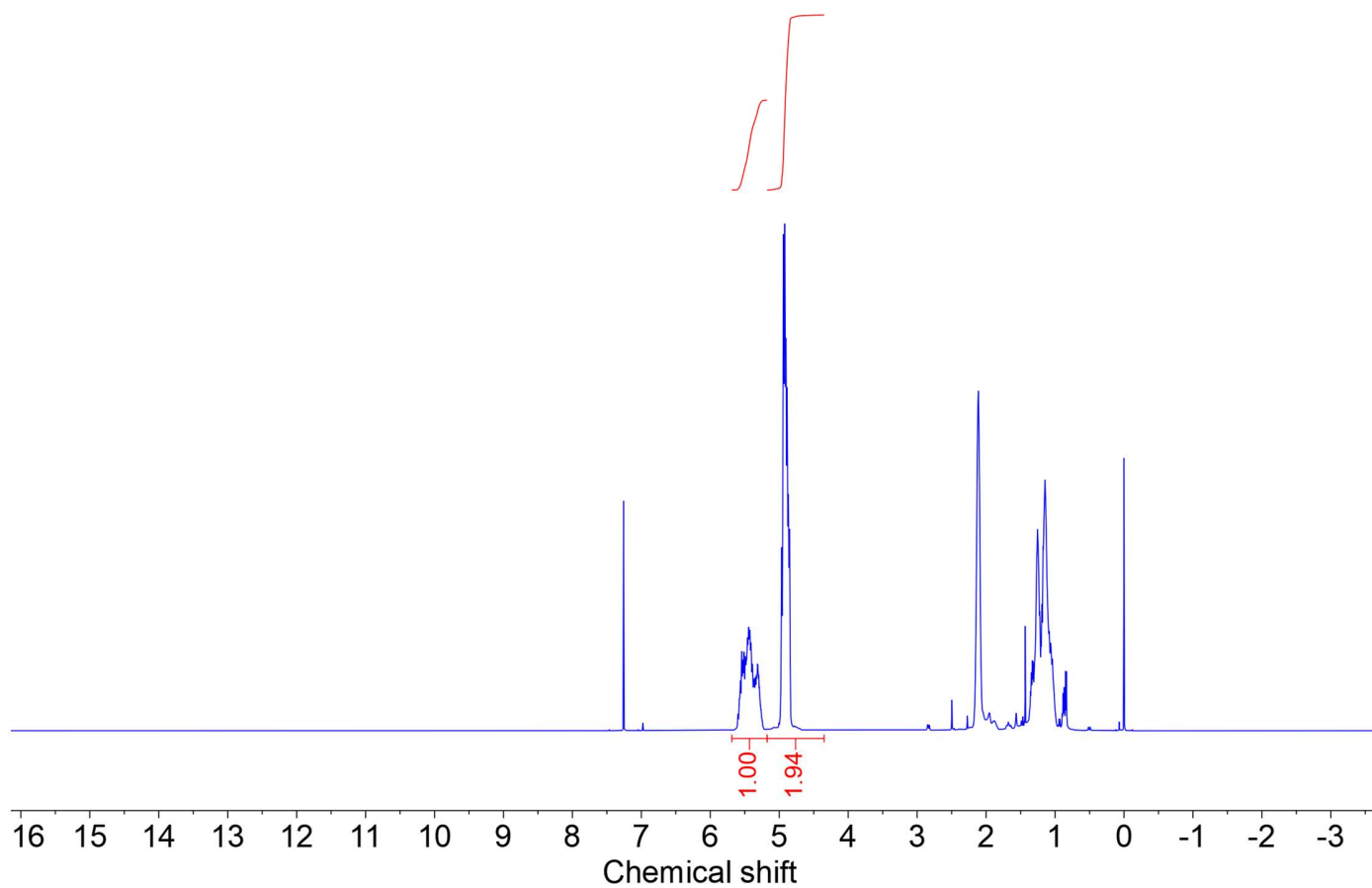


Figure S106. ^1H NMR spectrum of polybutadiene (**8** MeDiPip as ligand, polymerization at 0°C . 500 MHz, chloroform-d).

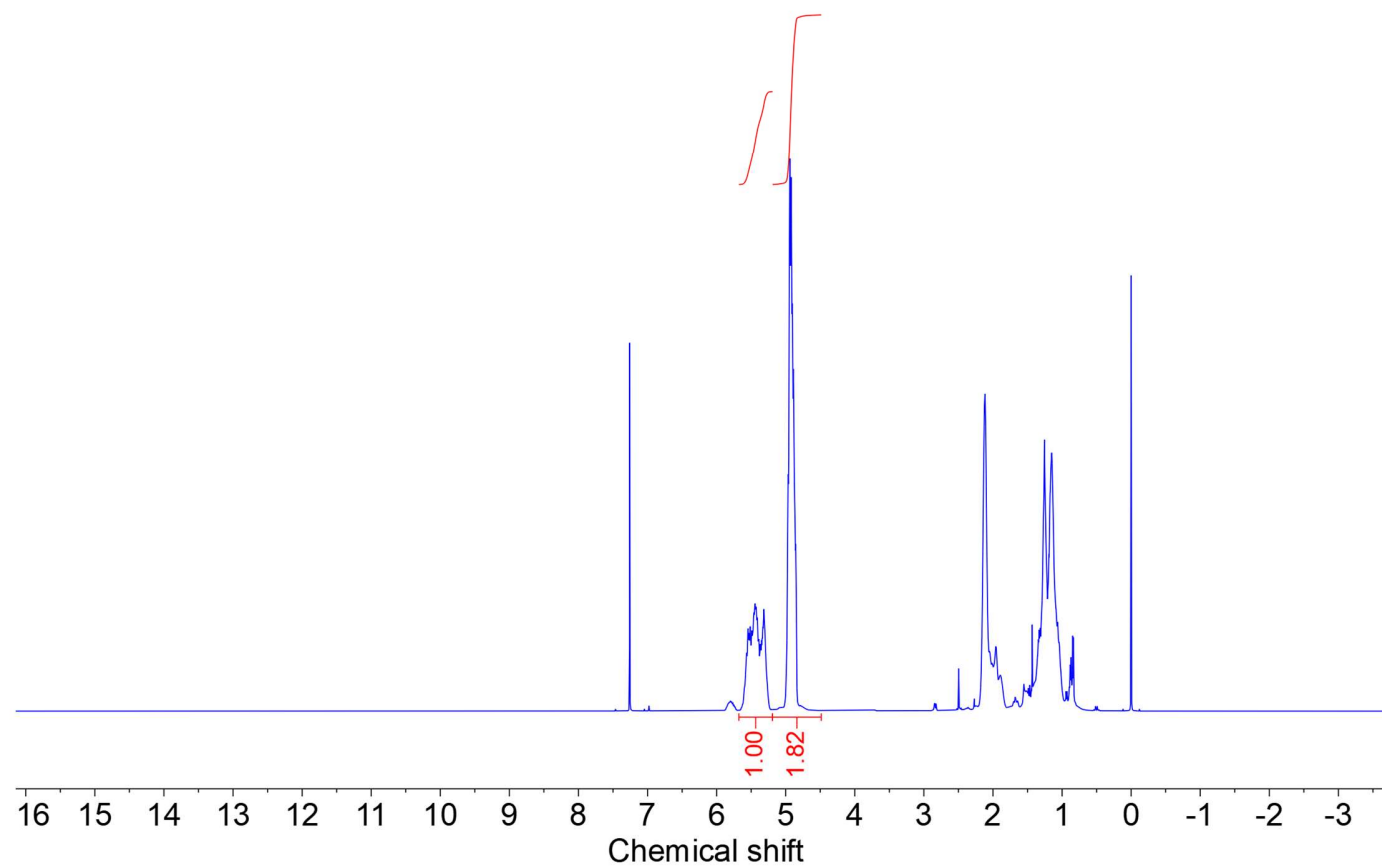


Figure S107. ^1H NMR spectrum of polybutadiene (**8** MeDiPip as ligand, polymerization at 40°C. 500 MHz, chloroform-d).

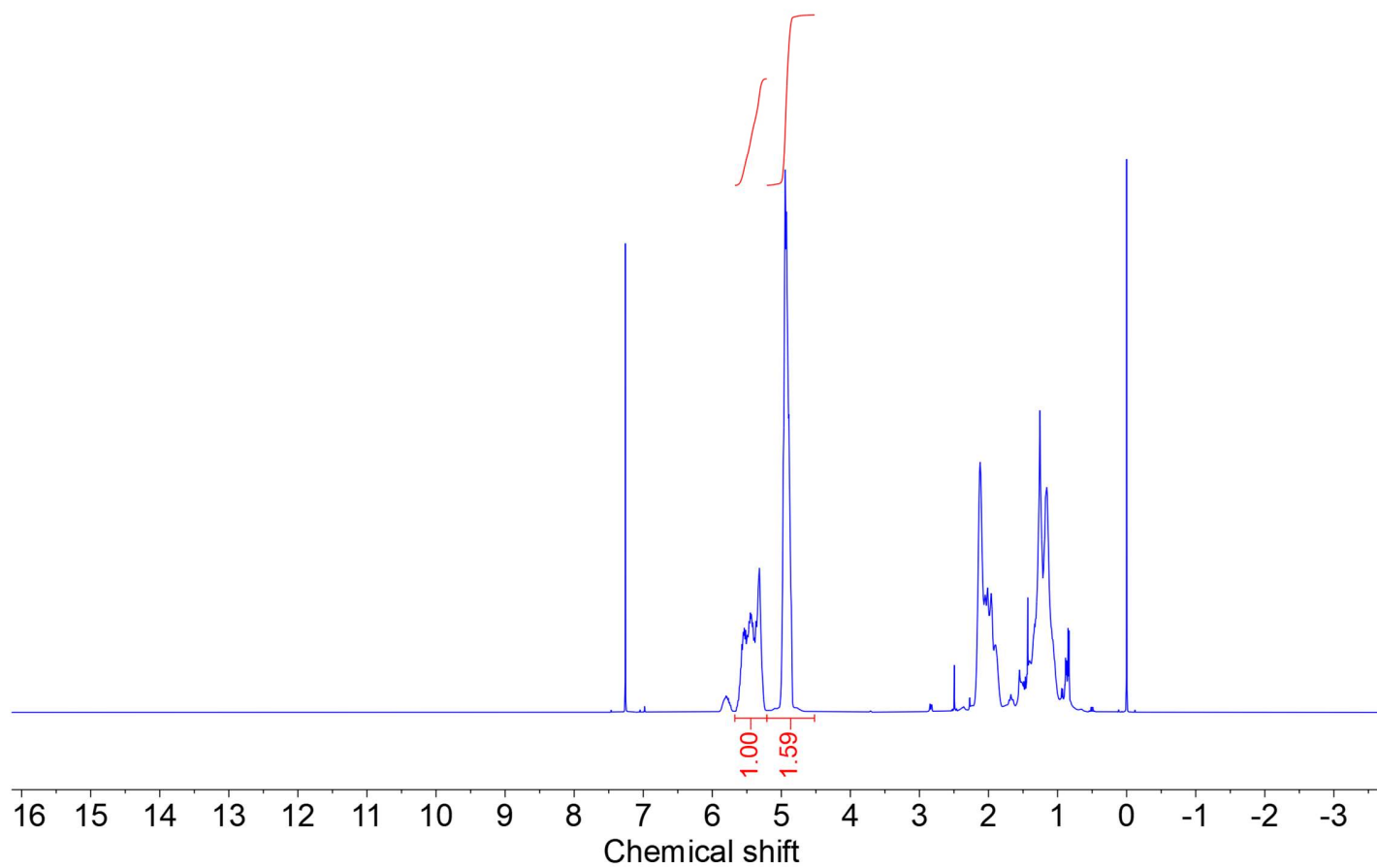


Figure S108. ^1H NMR spectrum of polybutadiene (**8** MeDiPip as ligand, polymerization at 60°C. 500 MHz, chloroform-d).

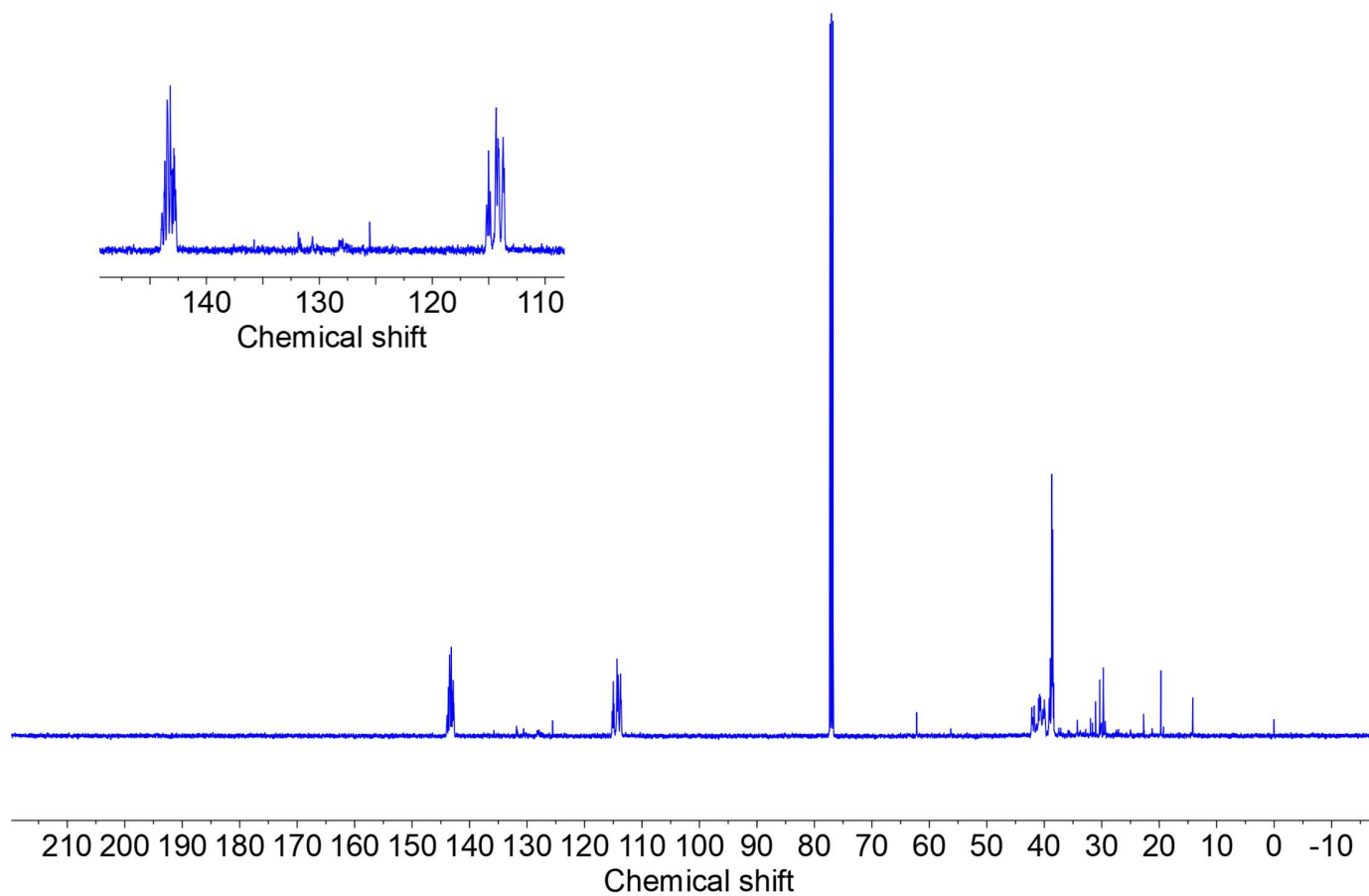


Figure S109. ^{13}C NMR spectrum of polybutadiene (**8** MeDiPip as ligand, polymerization at 20°C. 500 MHz, chloroform-d).

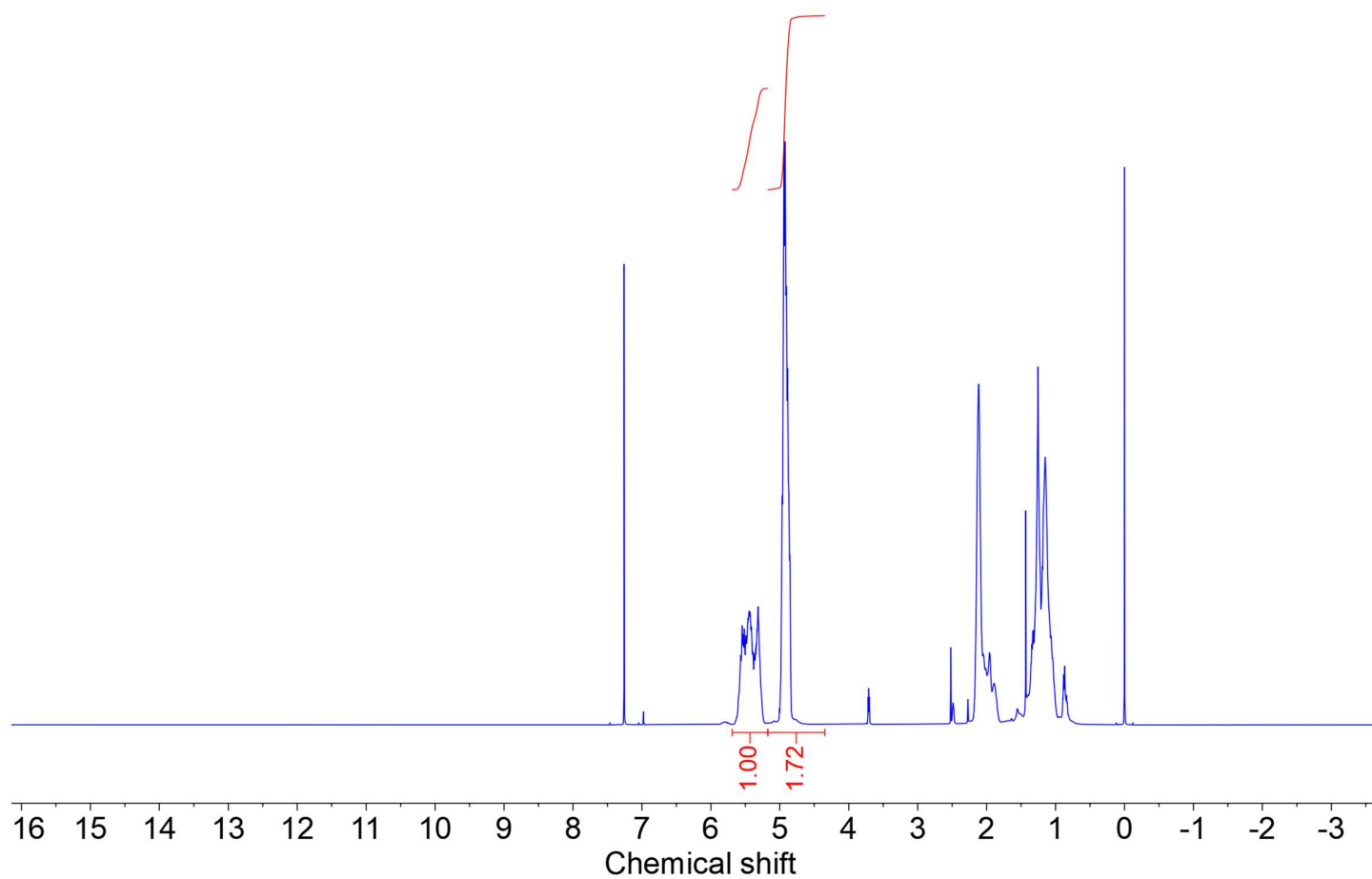


Figure S110. ^1H NMR spectrum of polybutadiene (**9** DiMph as ligand, polymerization at 20°C. 500 MHz, chloroform-d).

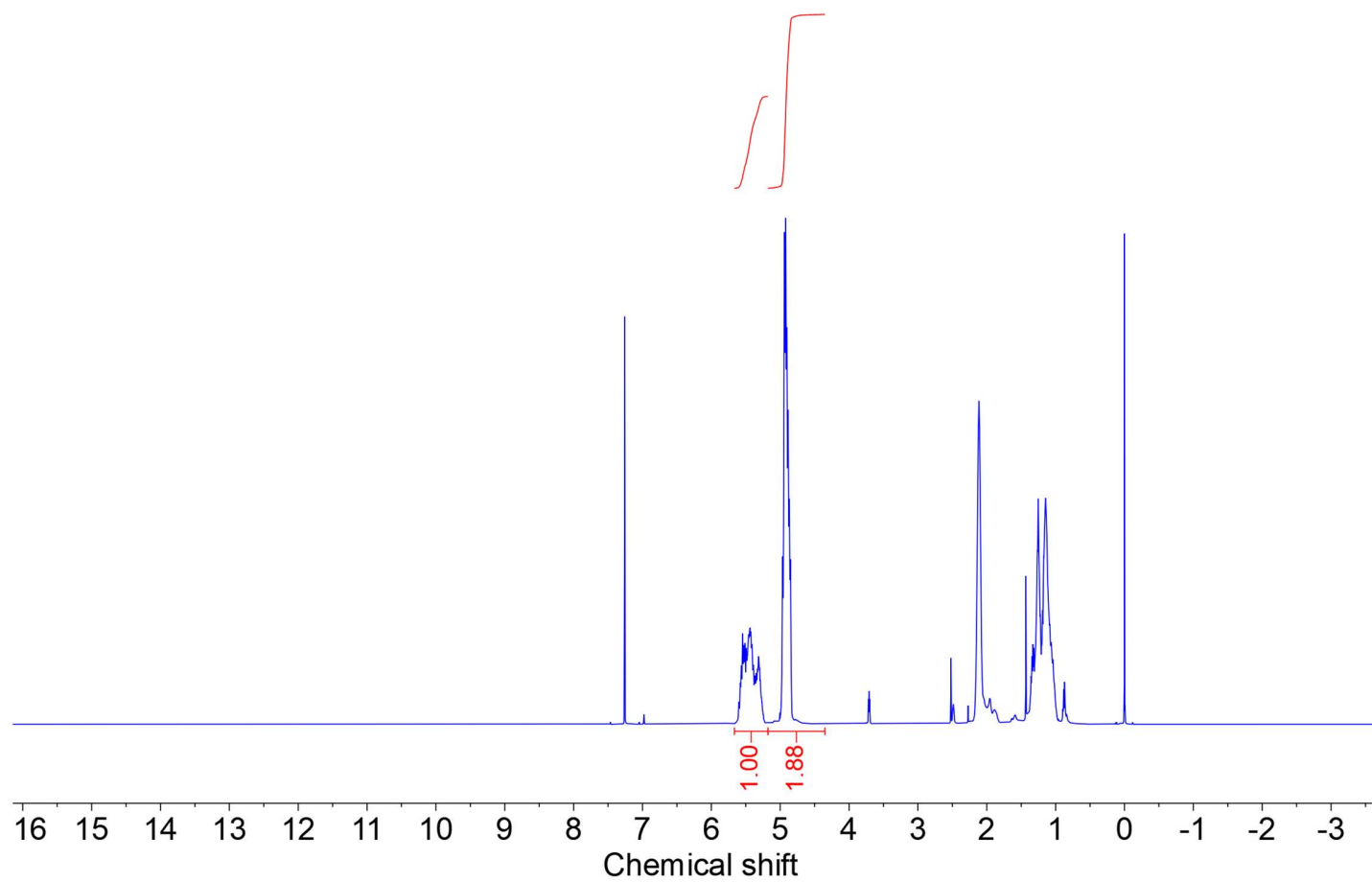


Figure S111. ^1H NMR spectrum of polybutadiene (**9** DiMph as ligand, polymerization at 0°C . 500 MHz, chloroform-d).

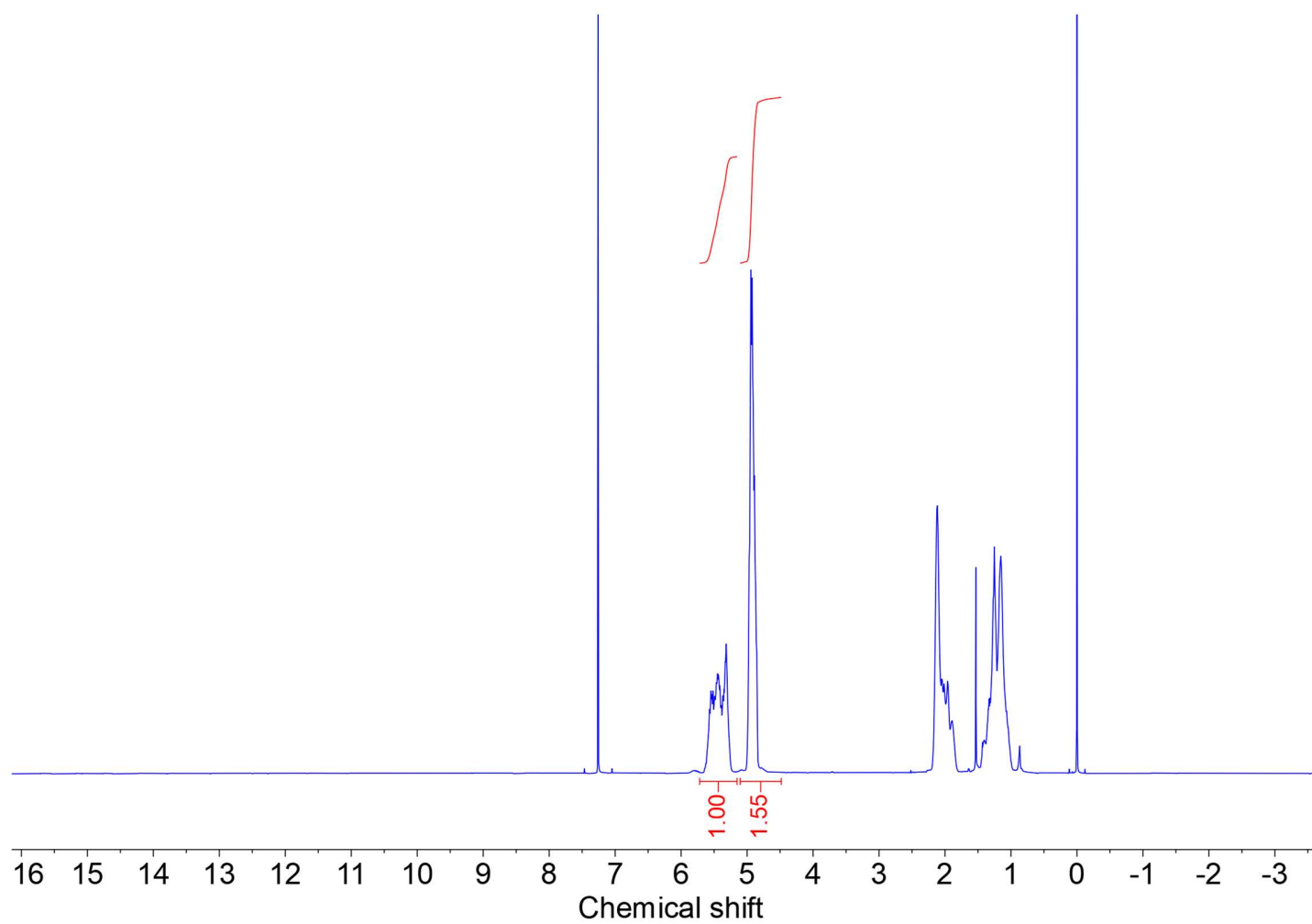


Figure S112. ^1H NMR spectrum of polybutadiene (**9** DiMph as ligand, polymerization at 40°C. 500 MHz, chloroform-d).

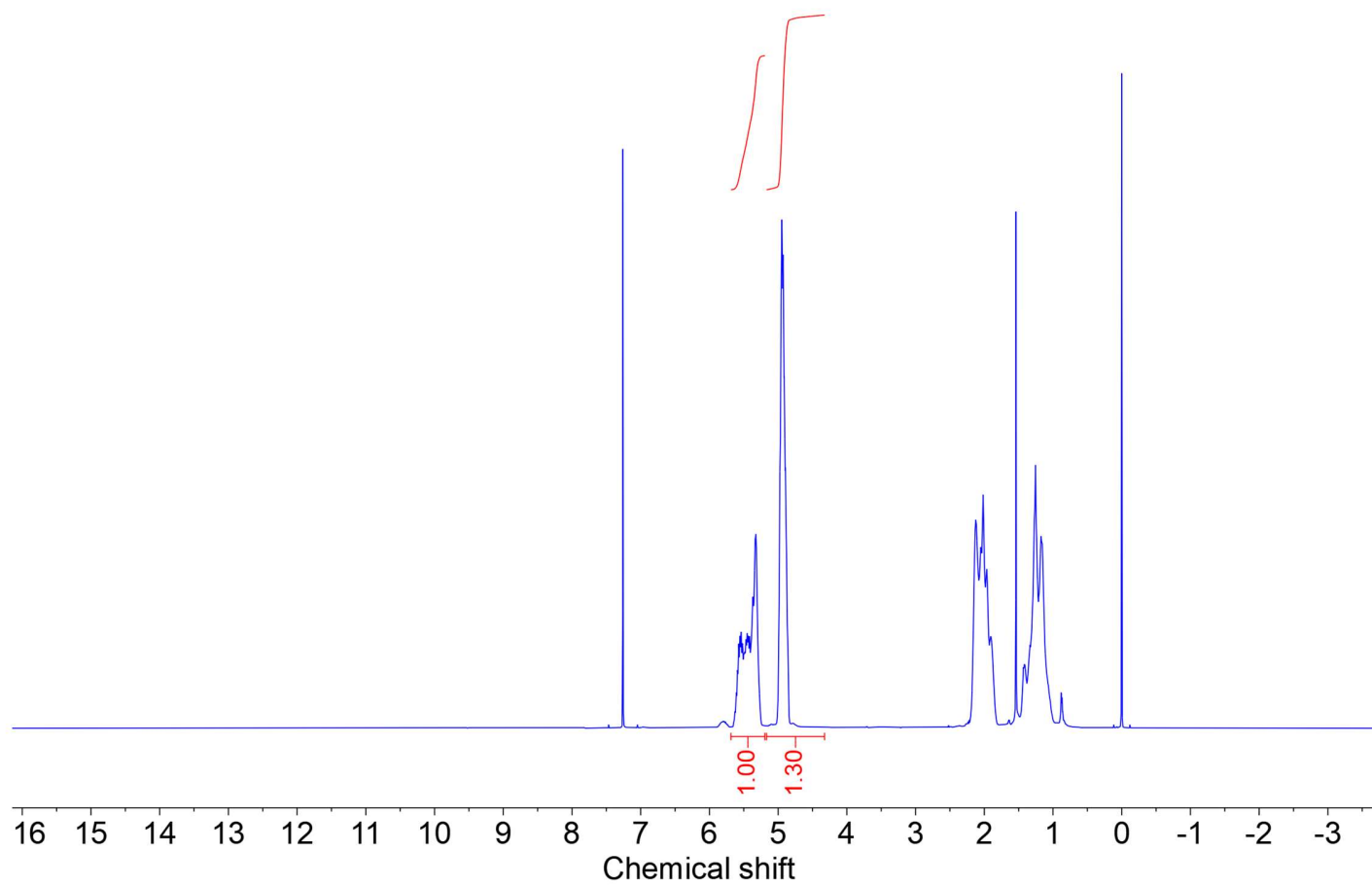


Figure S113. ^1H NMR spectrum of polybutadiene (**9** DiMph as ligand, polymerization at 60°C. 500 MHz, chloroform-d).

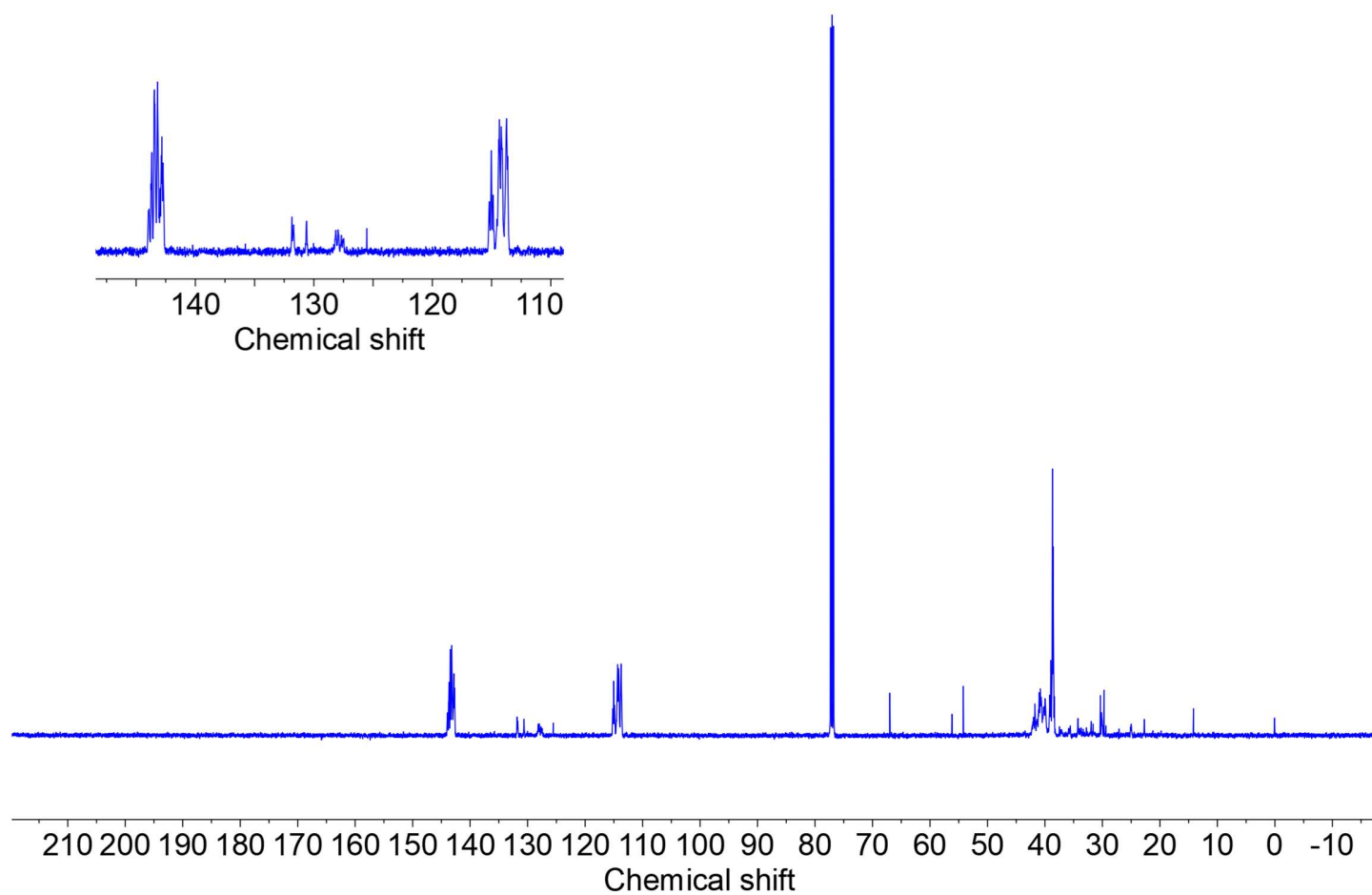


Figure S114. ^{13}C NMR spectrum of polybutadiene (**9** DiMph as ligand, polymerization at 20°C. 500 MHz, chloroform-d).

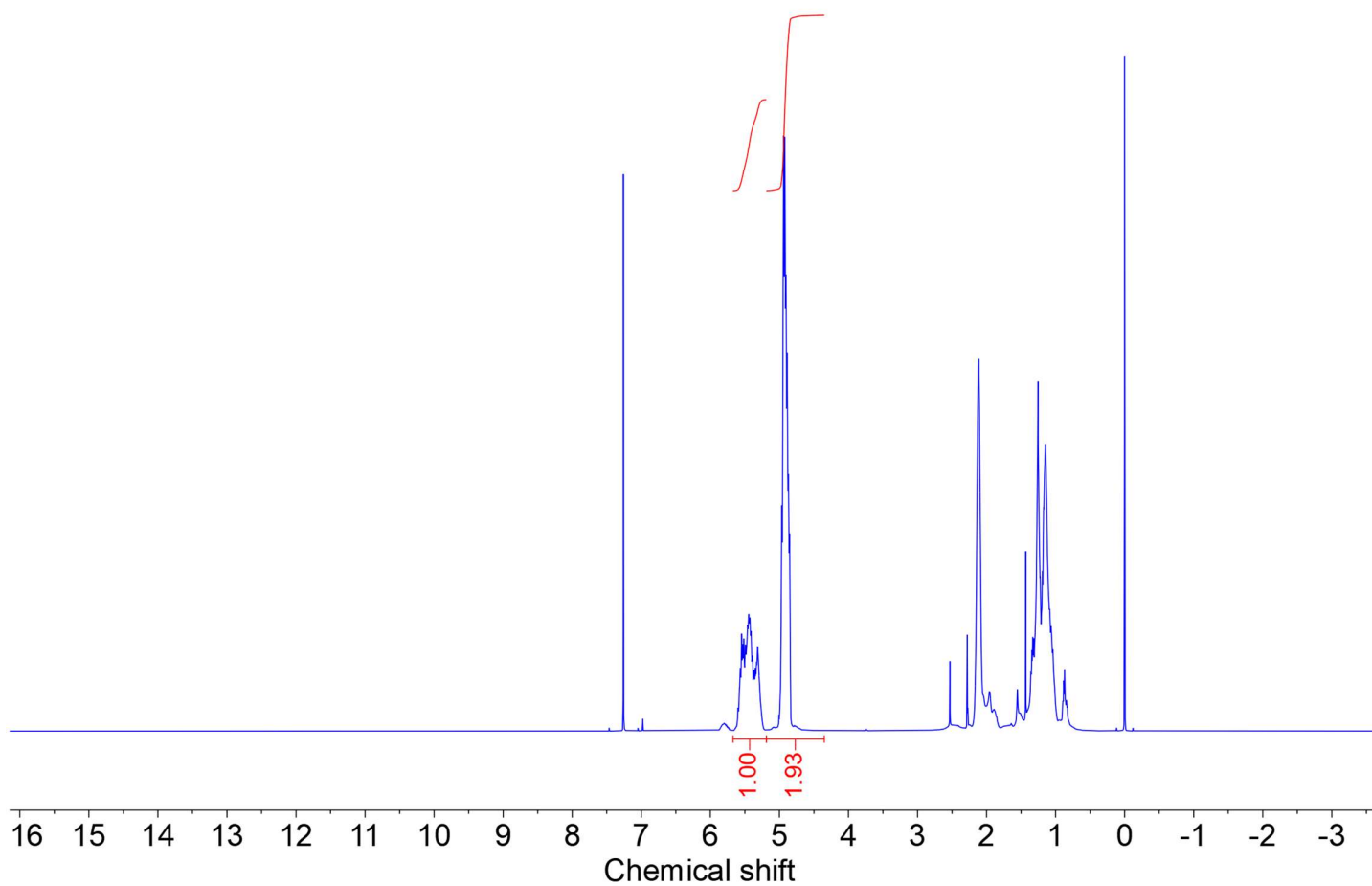


Figure S115. ^1H NMR spectrum of polybutadiene (**10** MeDiPz as ligand, polymerization at 20°C. 500 MHz, chloroform-d).

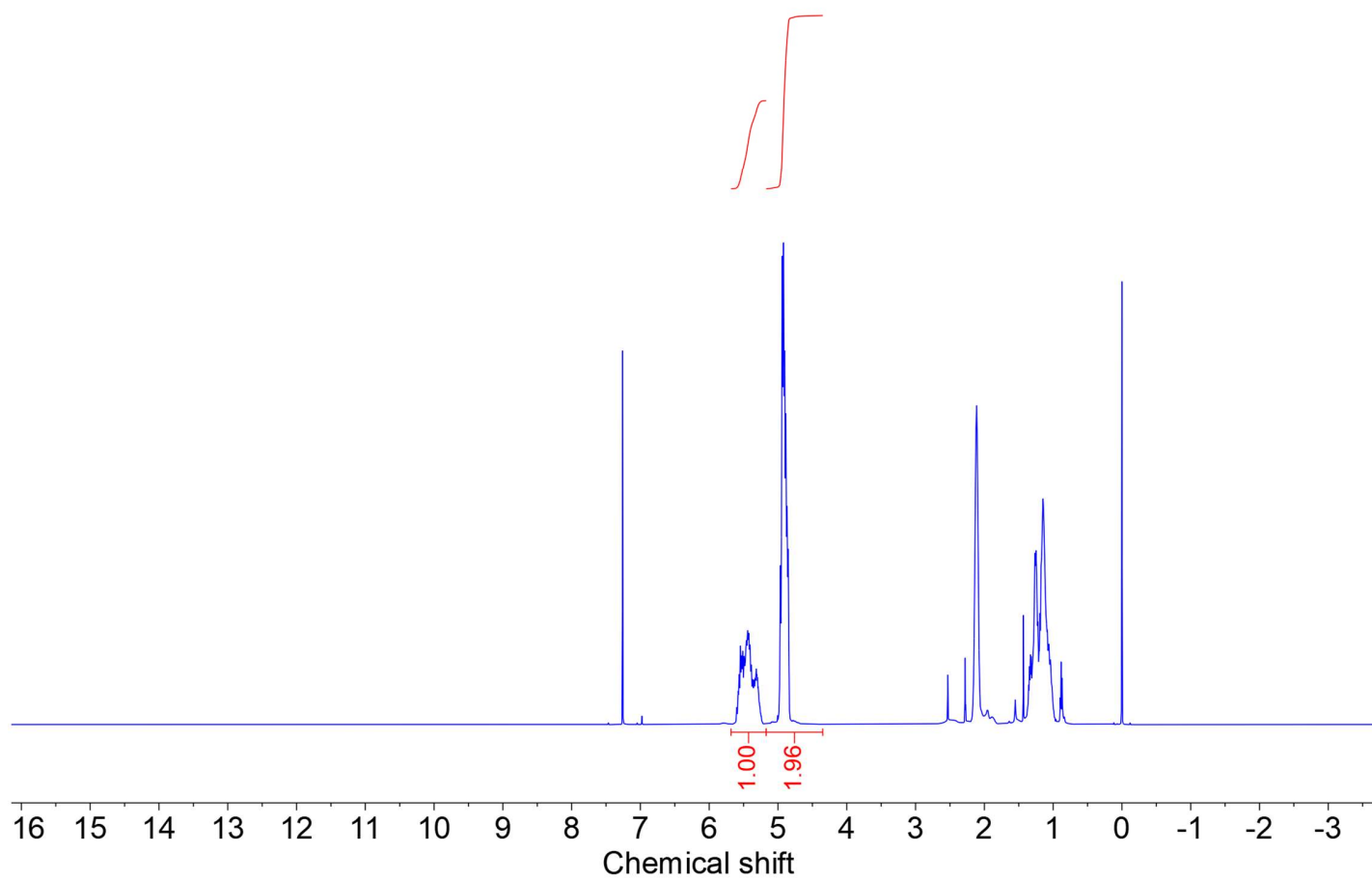


Figure S116. ^1H NMR spectrum of polybutadiene (**10** MeDiPz as ligand, polymerization at 0°C . 500 MHz, chloroform-d).

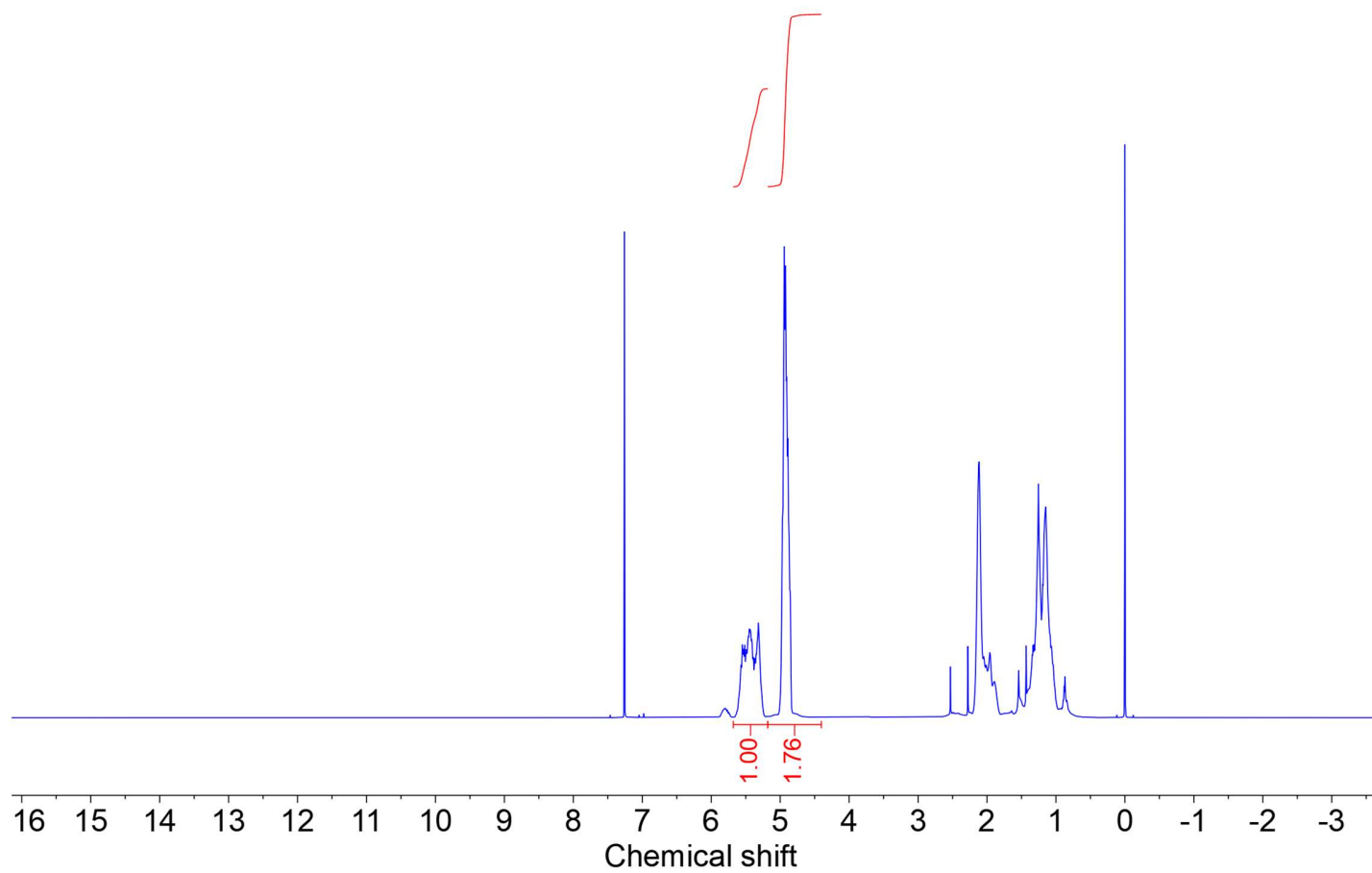


Figure S117. ^1H NMR spectrum of polybutadiene (**10** MeDiPz as ligand, polymerization at 40°C. 500 MHz, chloroform-d).

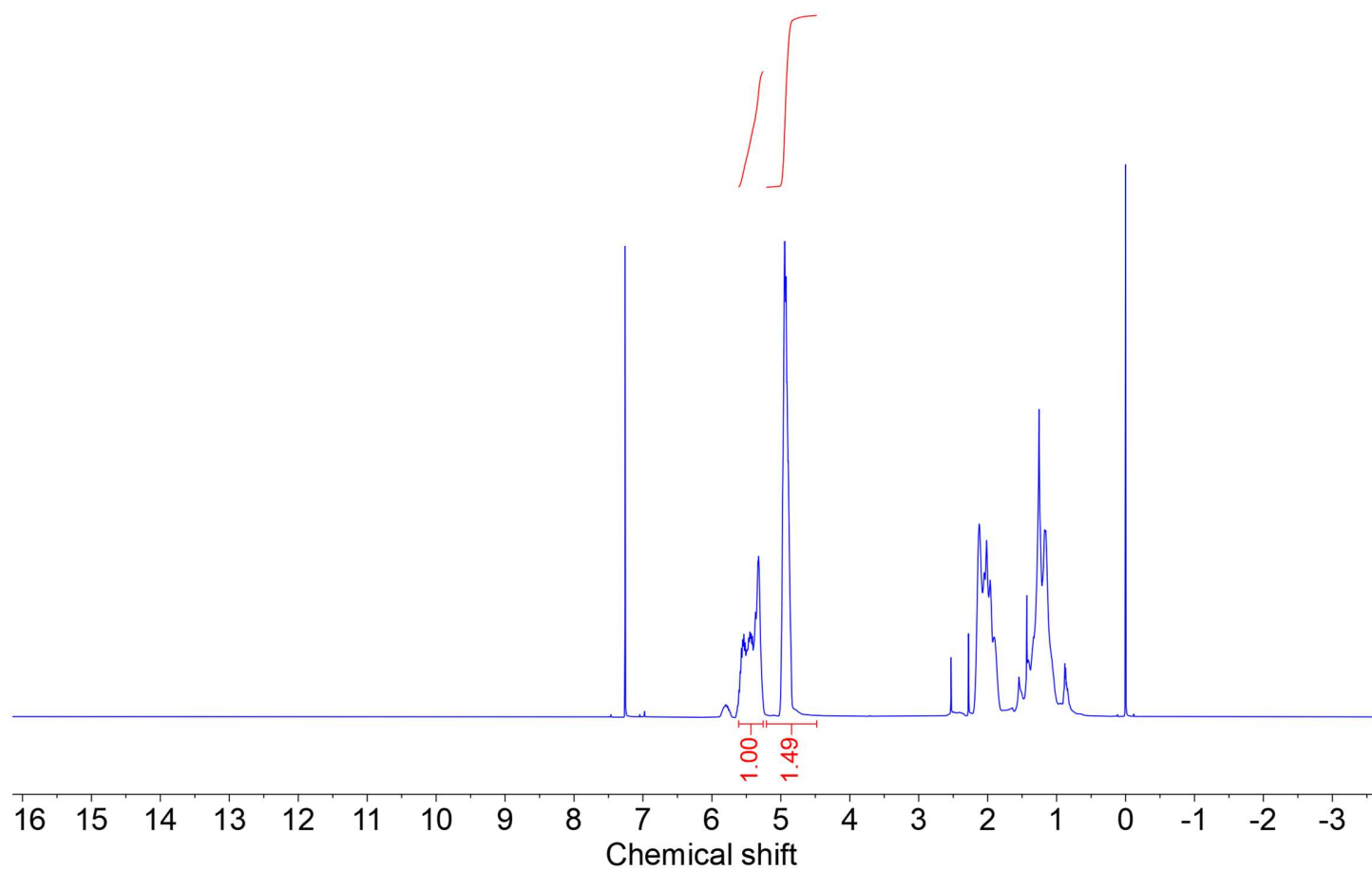


Figure S118. ^1H NMR spectrum of polybutadiene (**10** MeDiPz as ligand, polymerization at 60°C. 500 MHz, chloroform-d).

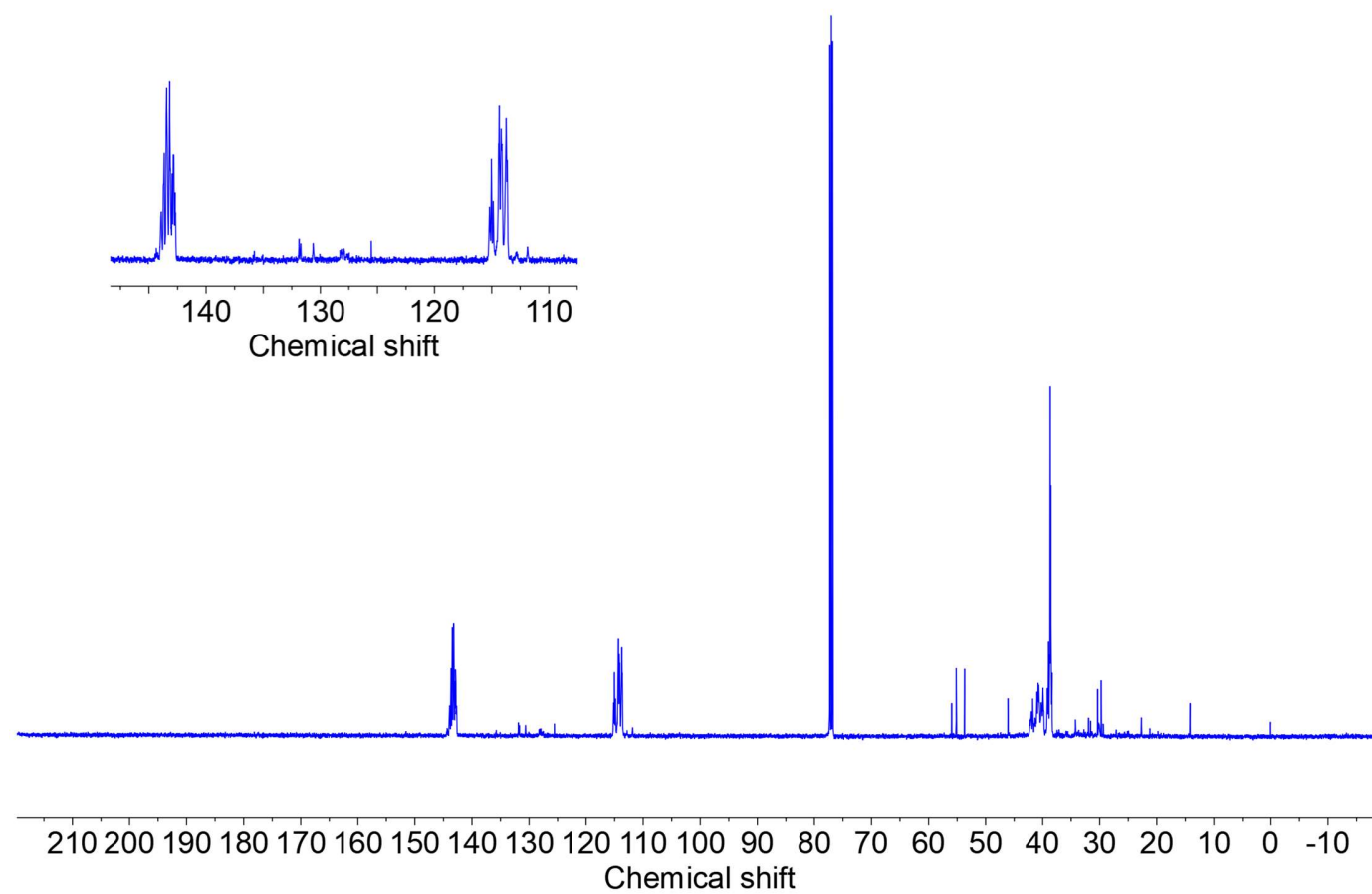


Figure S119. ^{13}C NMR spectrum of polybutadiene (**10** MeDiPz as ligand, polymerization at 20°C. 500 MHz, chloroform-d).

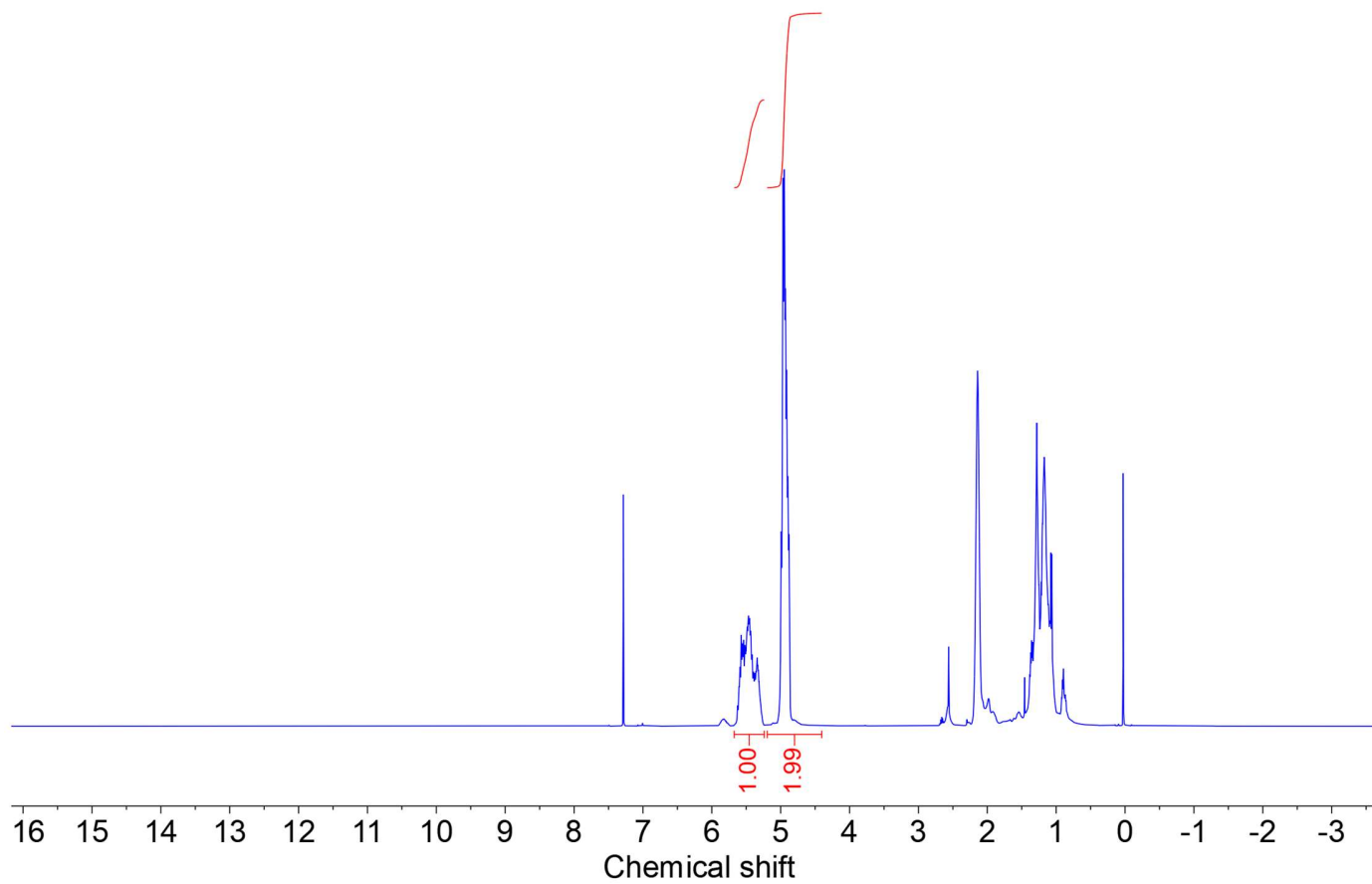


Figure S120. ^1H NMR spectrum of polybutadiene (**11** iPrDiPz as ligand, polymerization at 20°C. 500 MHz, chloroform-d).

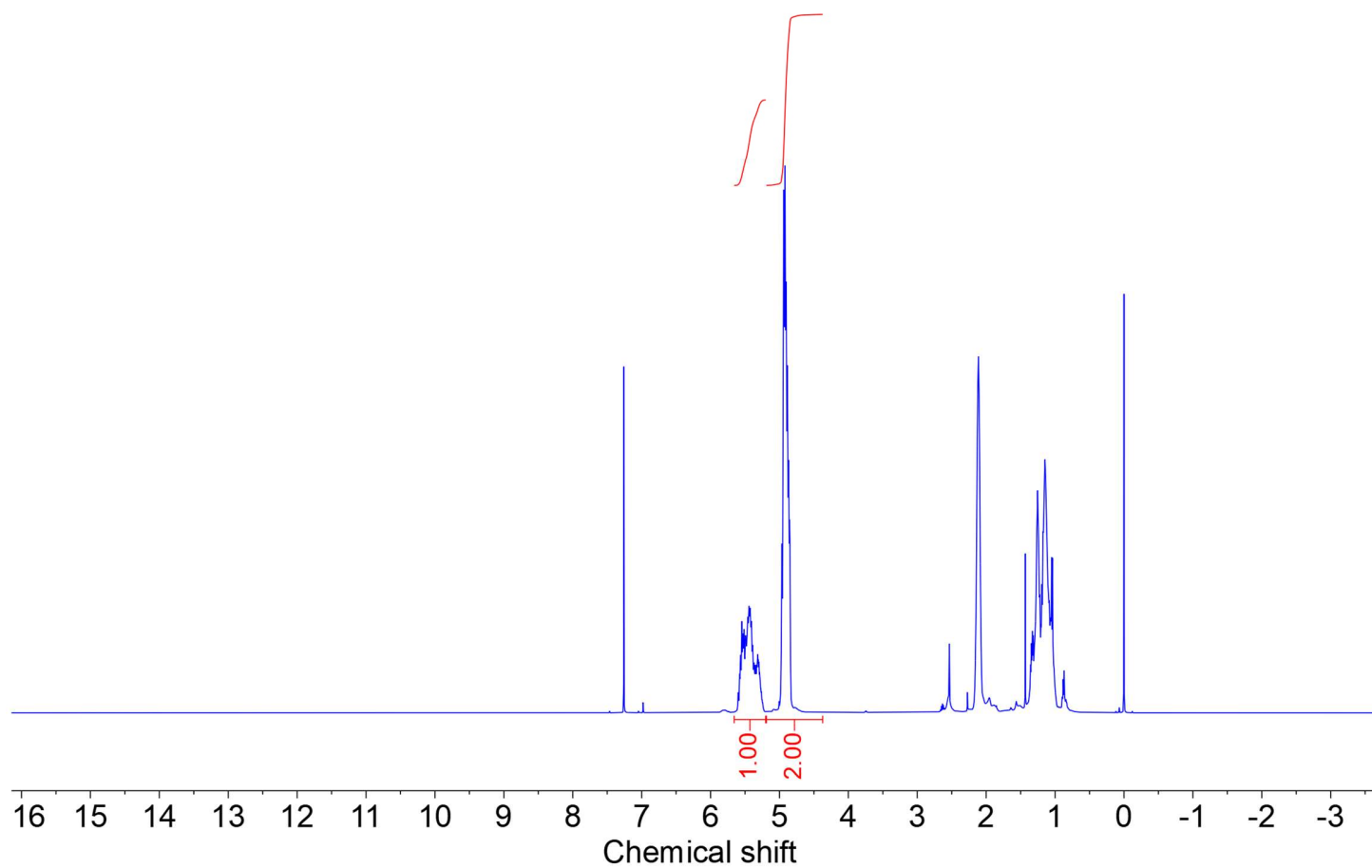


Figure S121. ^1H NMR spectrum of polybutadiene (**11** iPrDiPz as ligand, polymerization at 0°C . 500 MHz, chloroform-d).

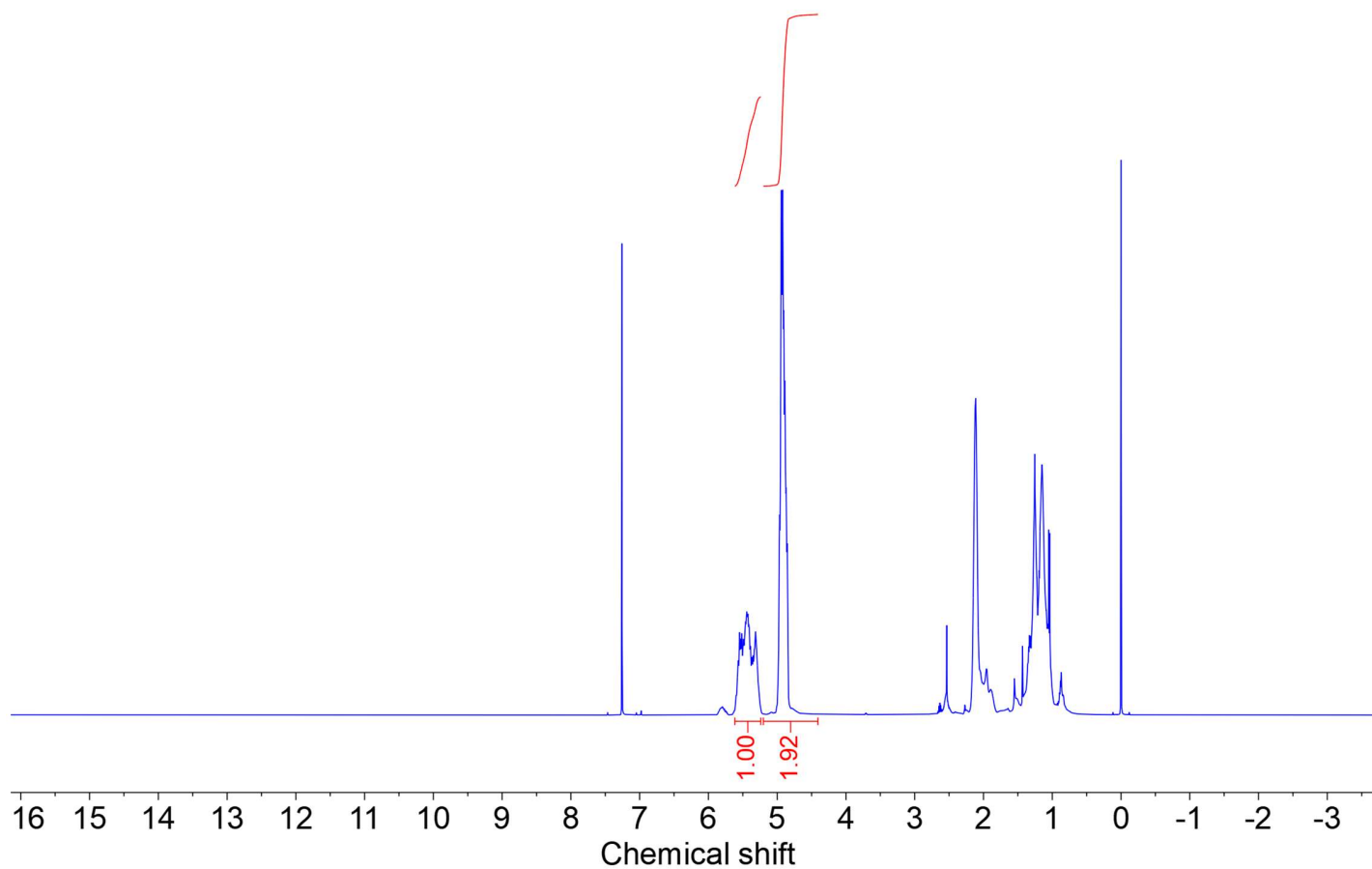


Figure S122. ^1H NMR spectrum of polybutadiene (**11** iPrDiPz as ligand, polymerization at 40°C . 500 MHz, chloroform-d).

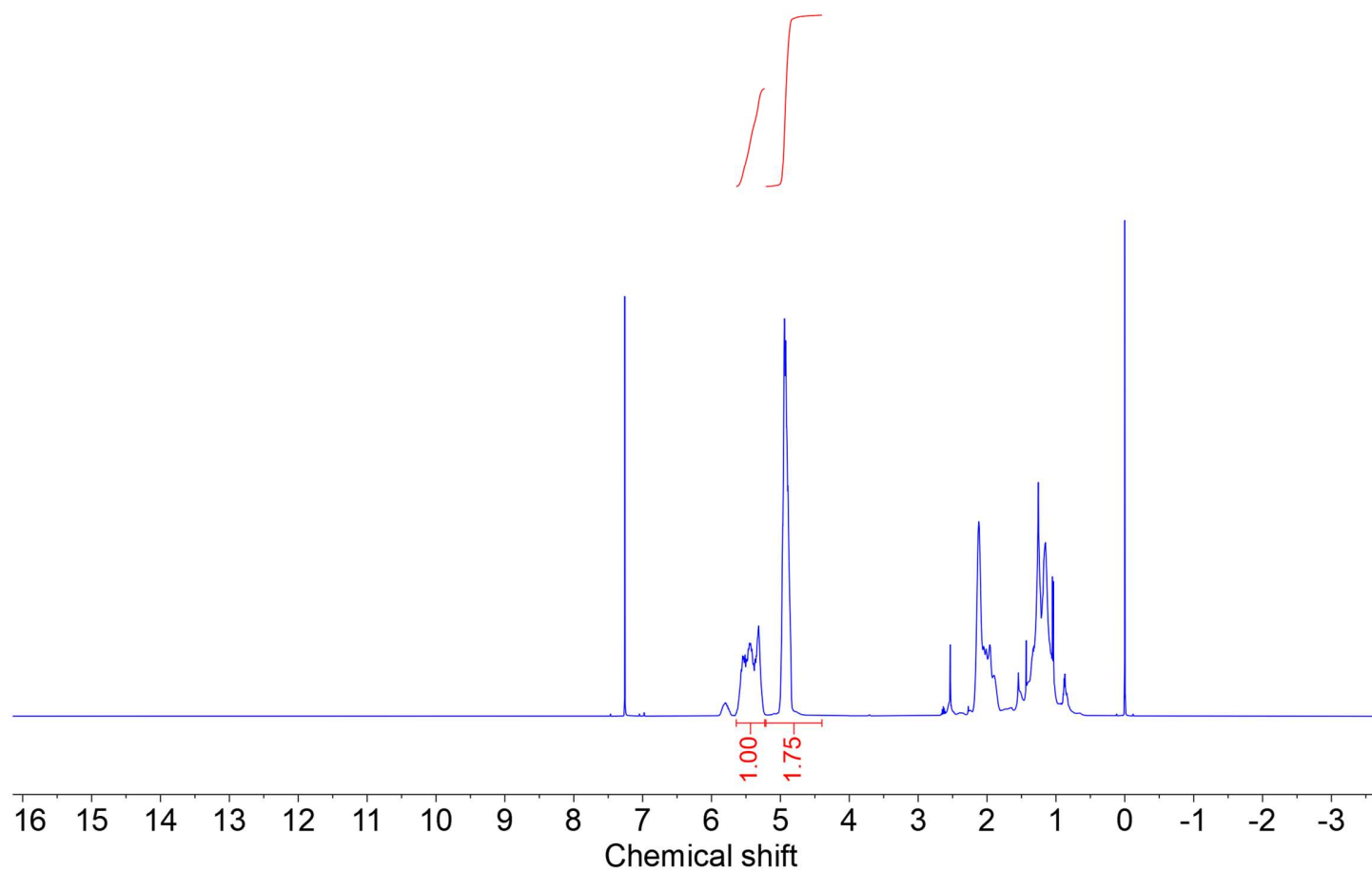


Figure S123. ^1H NMR spectrum of polybutadiene (**11** iPrDiPz as ligand, polymerization at 60°C. 500 MHz, chloroform-d).

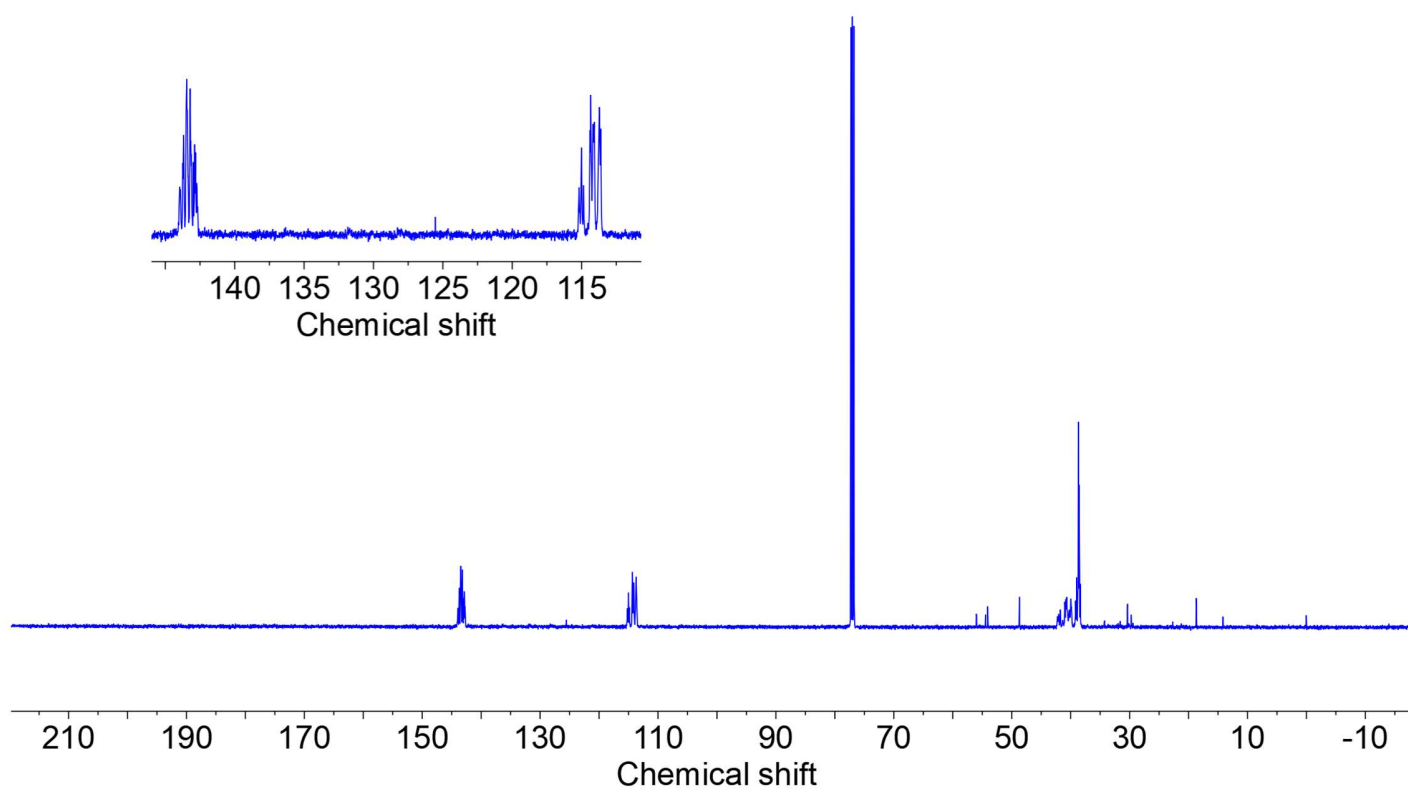


Figure S124. ^{13}C NMR spectrum of polybutadiene (**11** iPrDiPz as ligand, polymerization at 20°C. 500 MHz, chloroform-d).

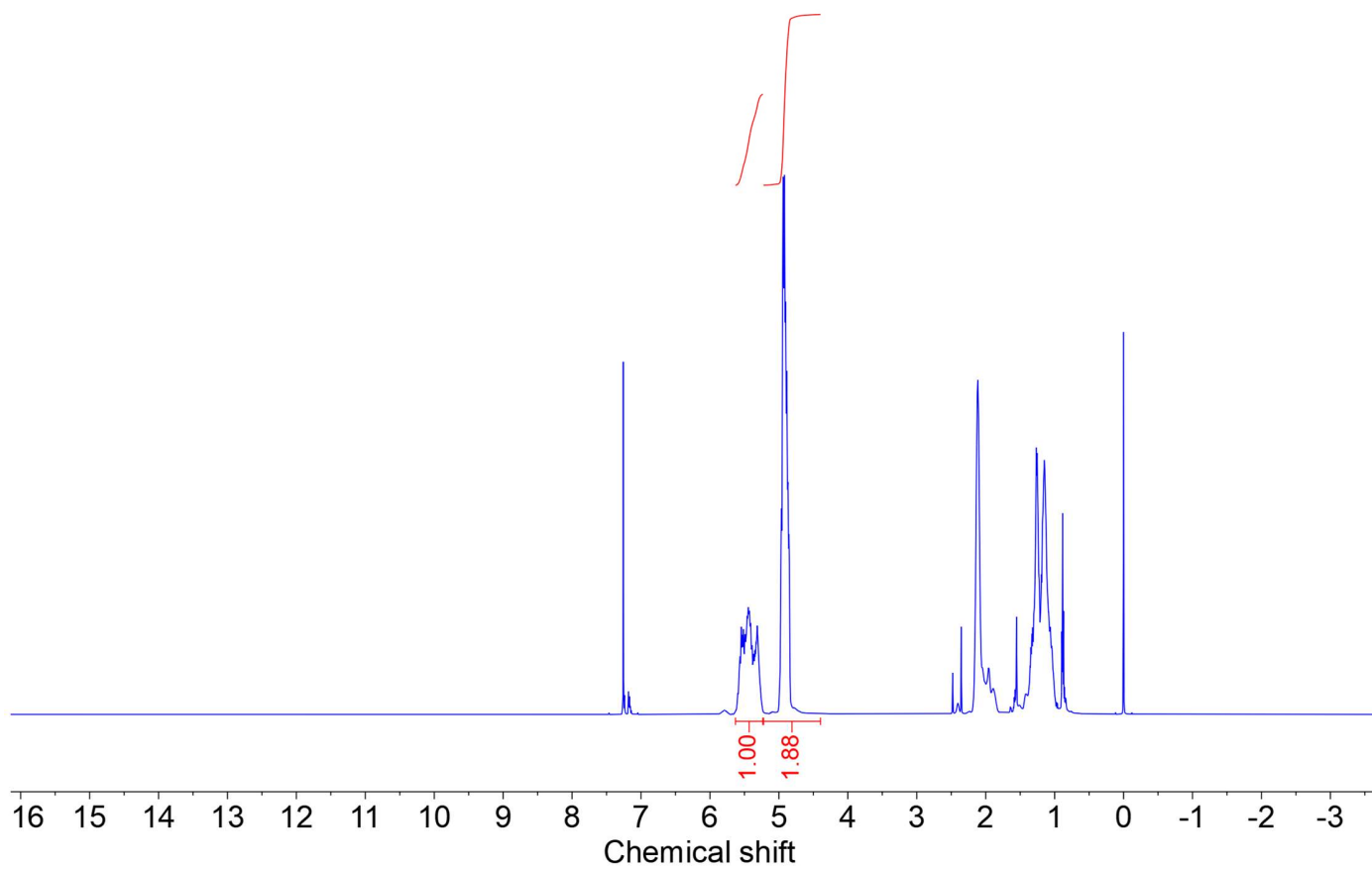


Figure S125. ^1H NMR spectrum of polybutadiene (Initiated by **6a** complex, polymerization at 20°C. 500 MHz, chloroform-d).

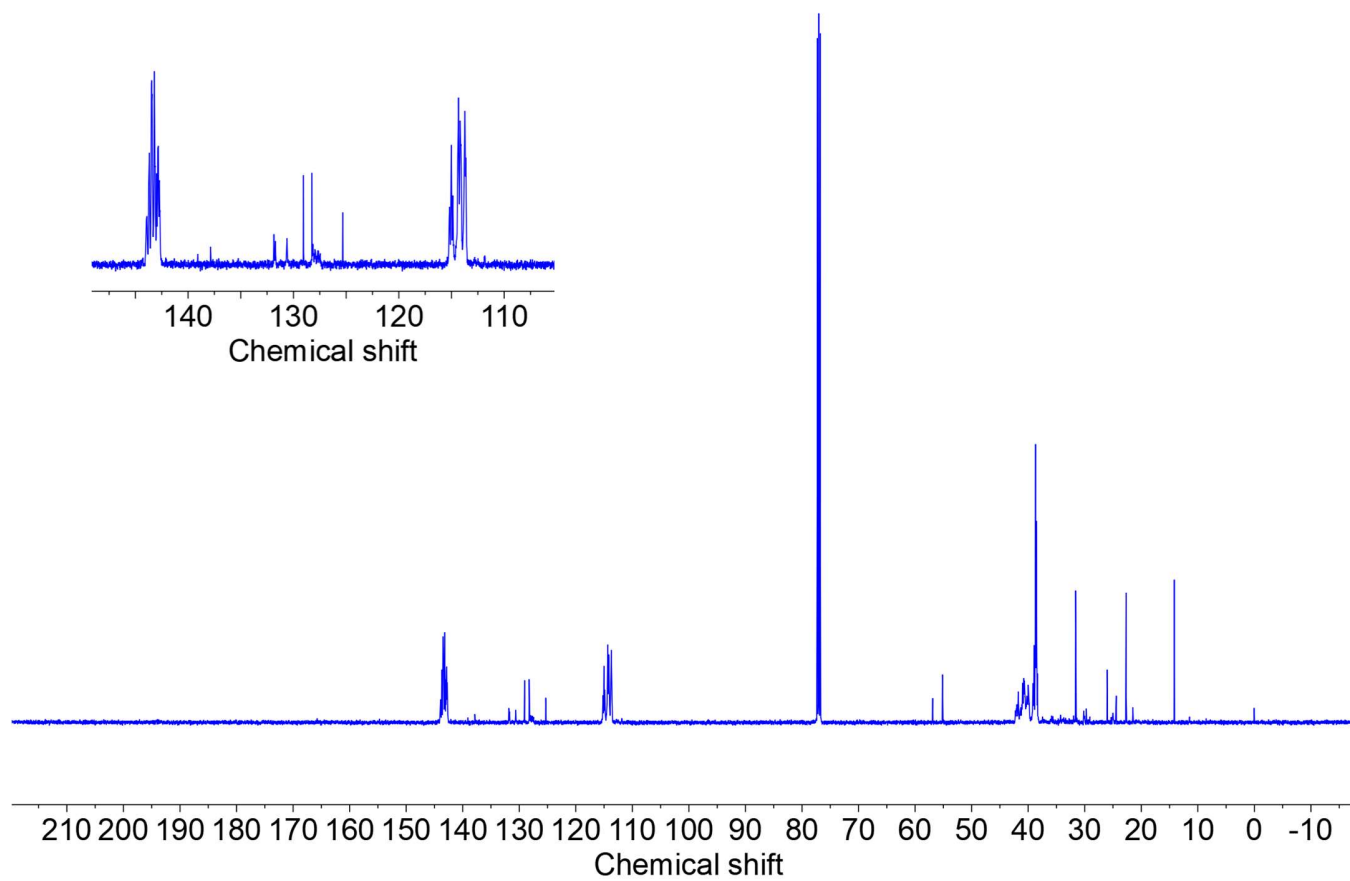


Figure S126. ^{13}C NMR spectrum of polybutadiene (Initiated by **6a** complex, polymerization at 20°C. 500 MHz, chloroform-d).

GPC Curve and Average Molecular Weight Data of the Polybutadiene

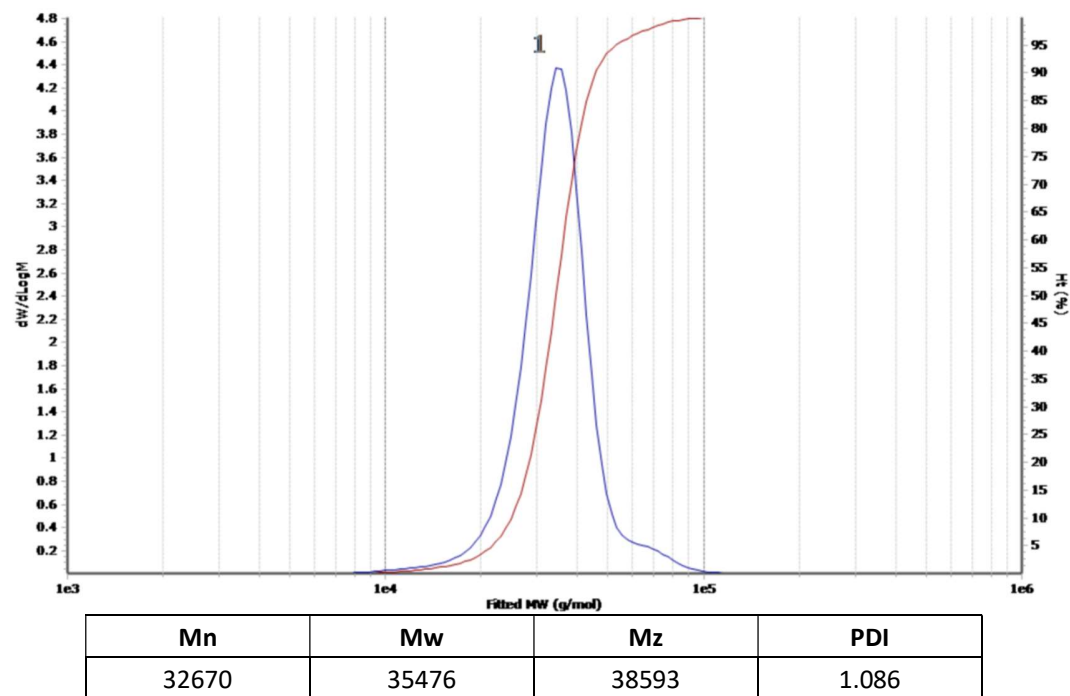


Figure S127. GPC curve and average molecular weight data of polybutadiene obtained by t-BuLi/**1** glyme (Table 1, entry 1).

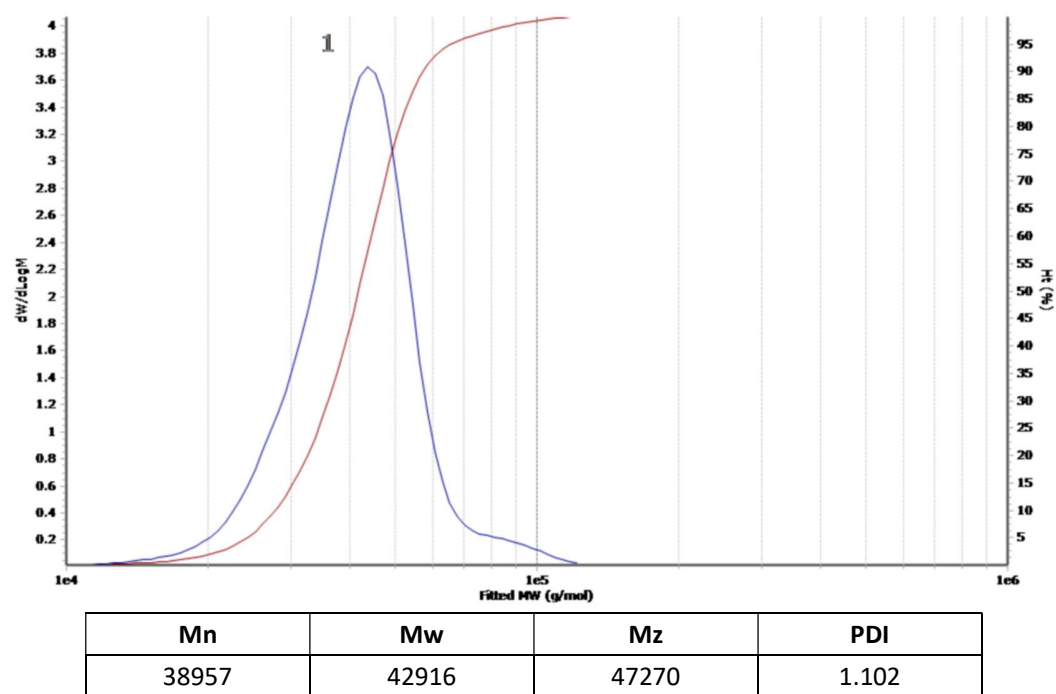


Figure S128. GPC curve and average molecular weight data of polybutadiene obtained by t-BuLi/2 THF (Table 1, entry 2).

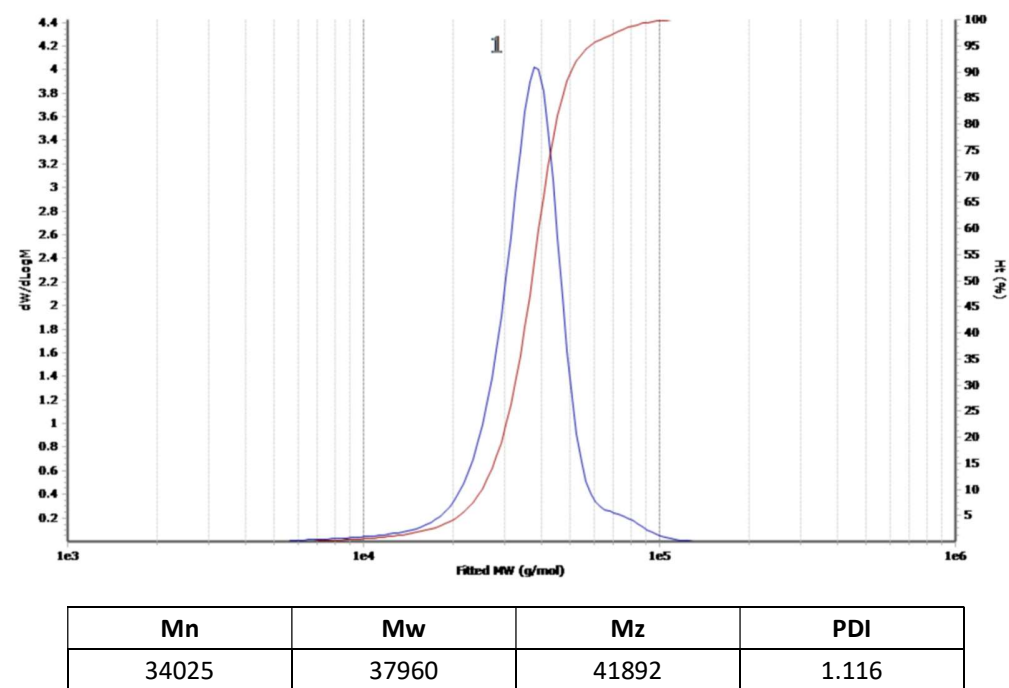


Figure S129. GPC curve and average molecular weight data of polybutadiene obtained by t-BuLi/3 TMEDA (Table 1, entry 3).

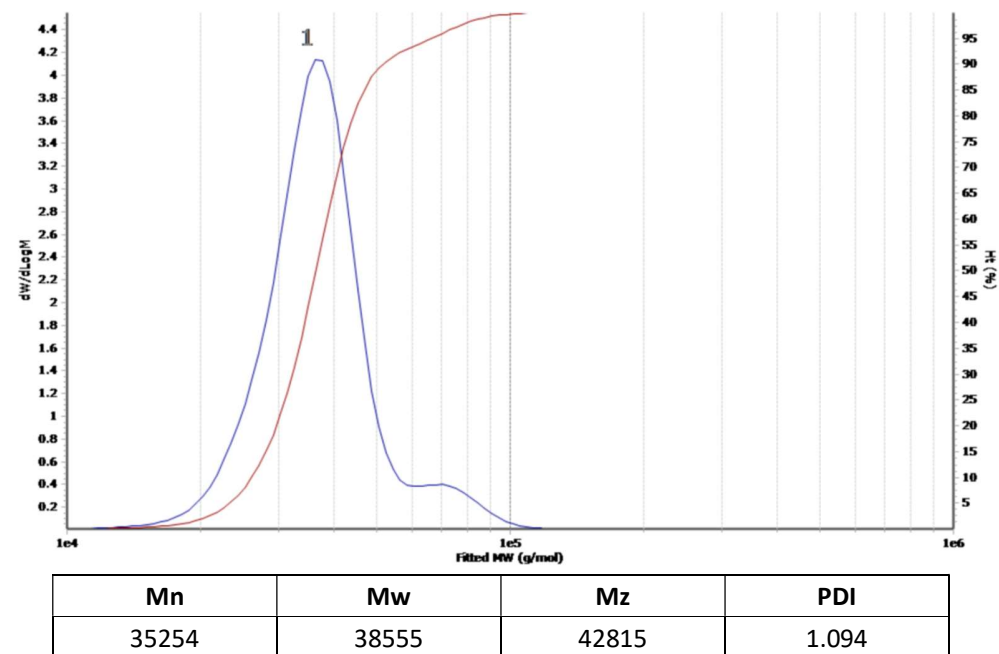


Figure S130. GPC curve and average molecular weight data of polybutadiene obtained by *t*-BuLi/**4** TEEDA (Table 1, entry 4).

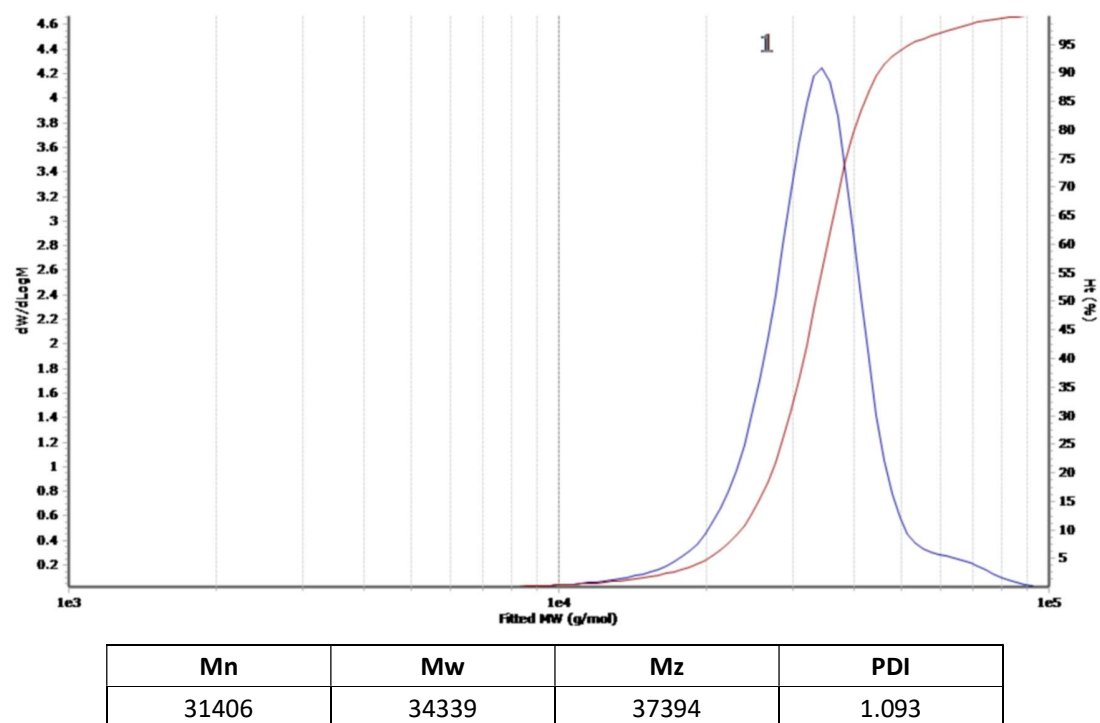
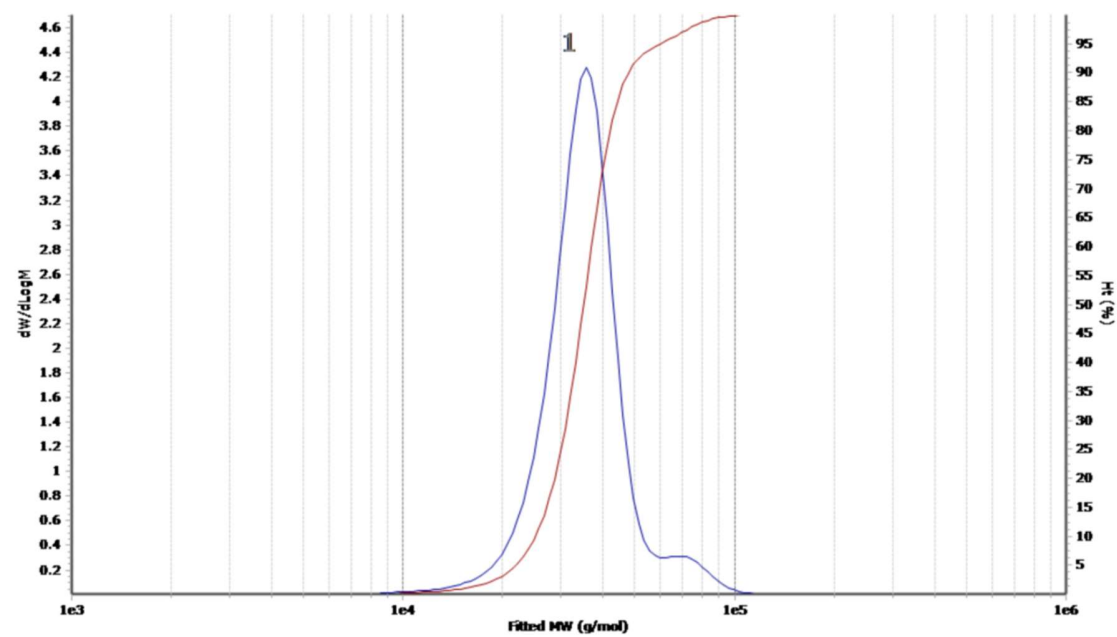


Figure S131. GPC curve and average molecular weight data of polybutadiene obtained by t-BuLi/5 DiPyr (Table 1, entry 5).



Mn	Mw	Mz	PDI
33496	36664	40478	1.095

Figure S132. GPC curve and average molecular weight data of polybutadiene obtained by t-BuLi/**6** DiPip (Table 1, entry 6).

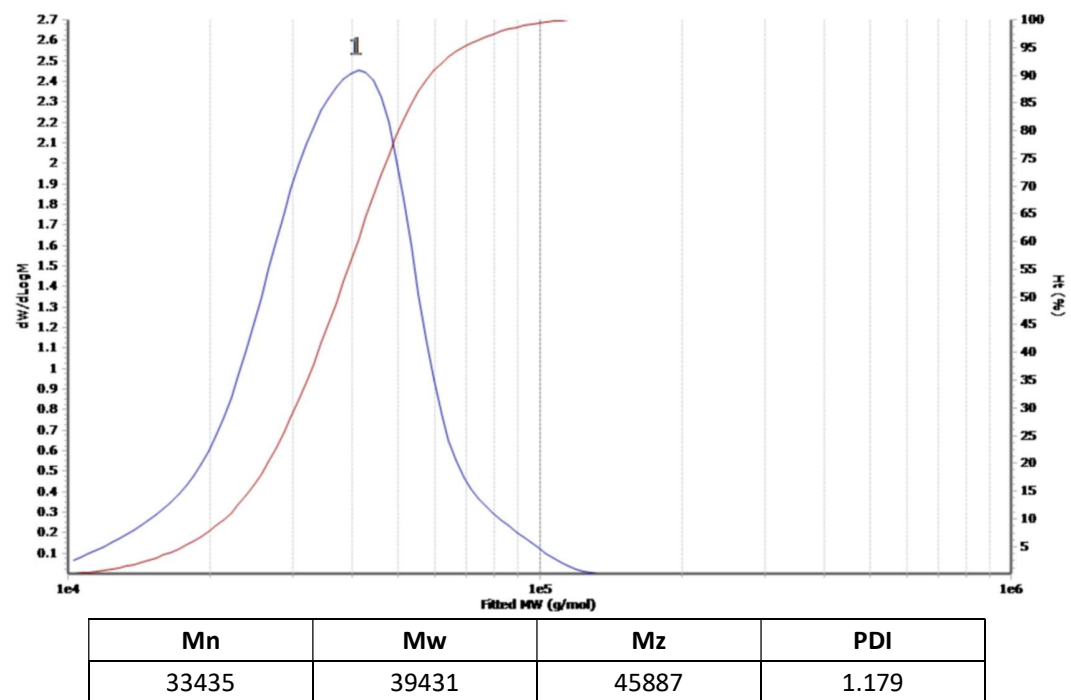


Figure S133. GPC curve and average molecular weight data of polybutadiene obtained by t-BuLi/7 DiAze (Table 1, entry 7).

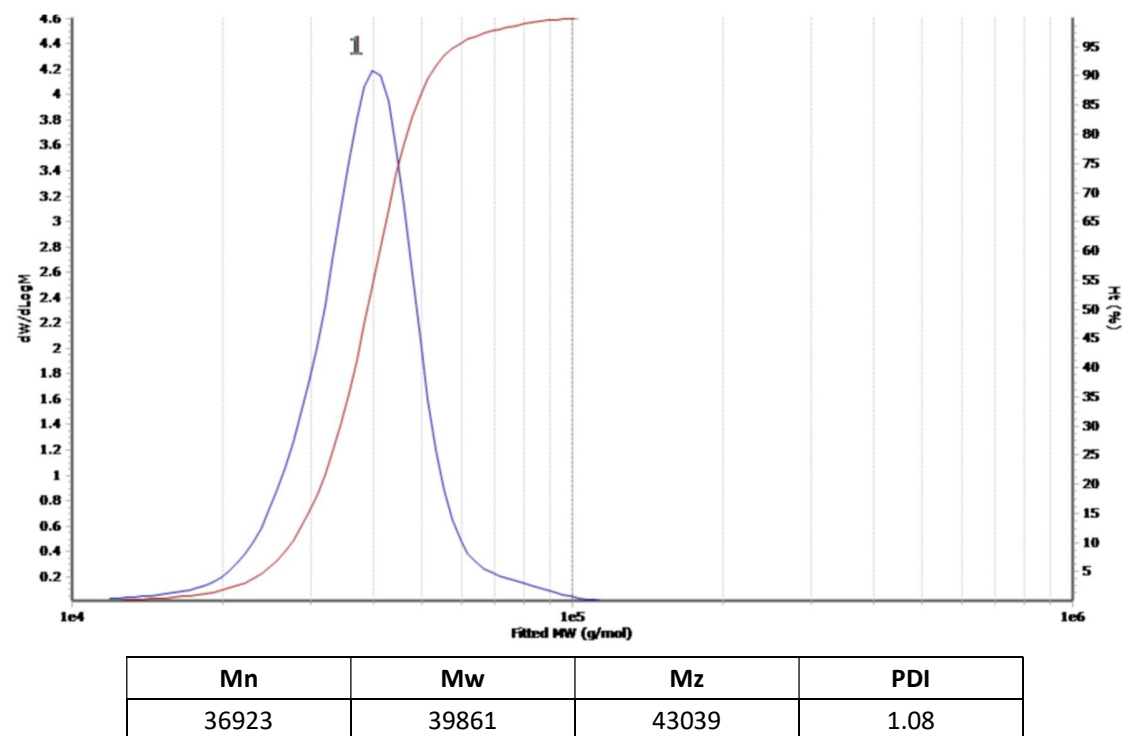


Figure S134. GPC curve and average molecular weight data of polybutadiene obtained by t-BuLi/**8** MeDiPip.

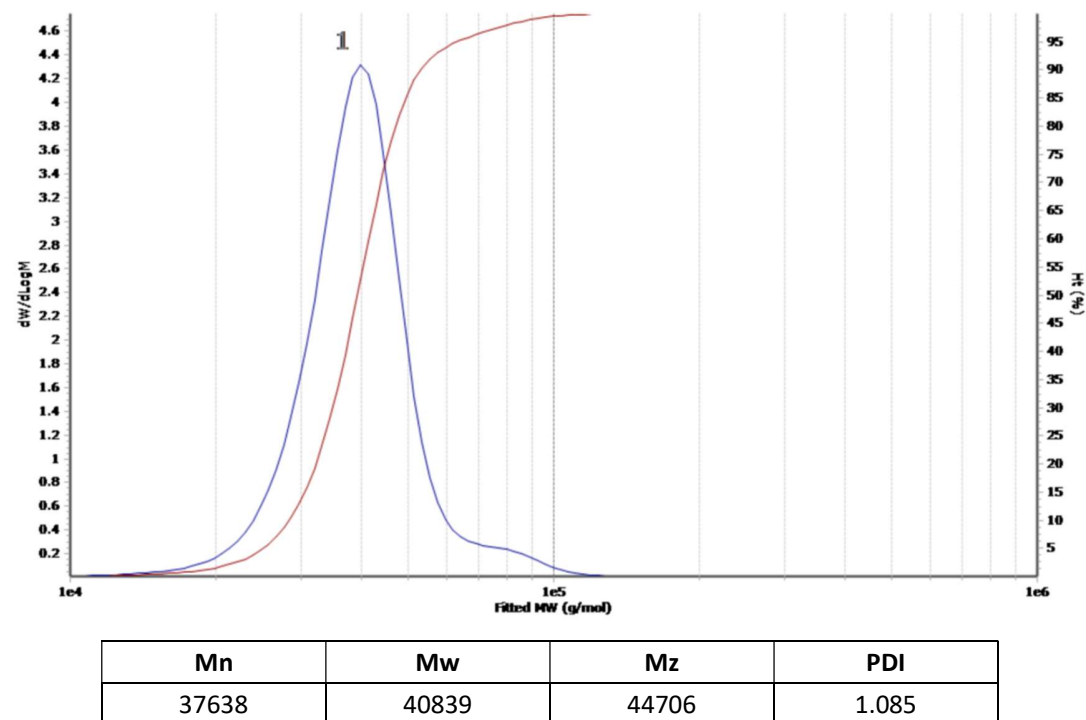


Figure S135. GPC curve and average molecular weight data of polybutadiene obtained by t-BuLi/9 DiMph.

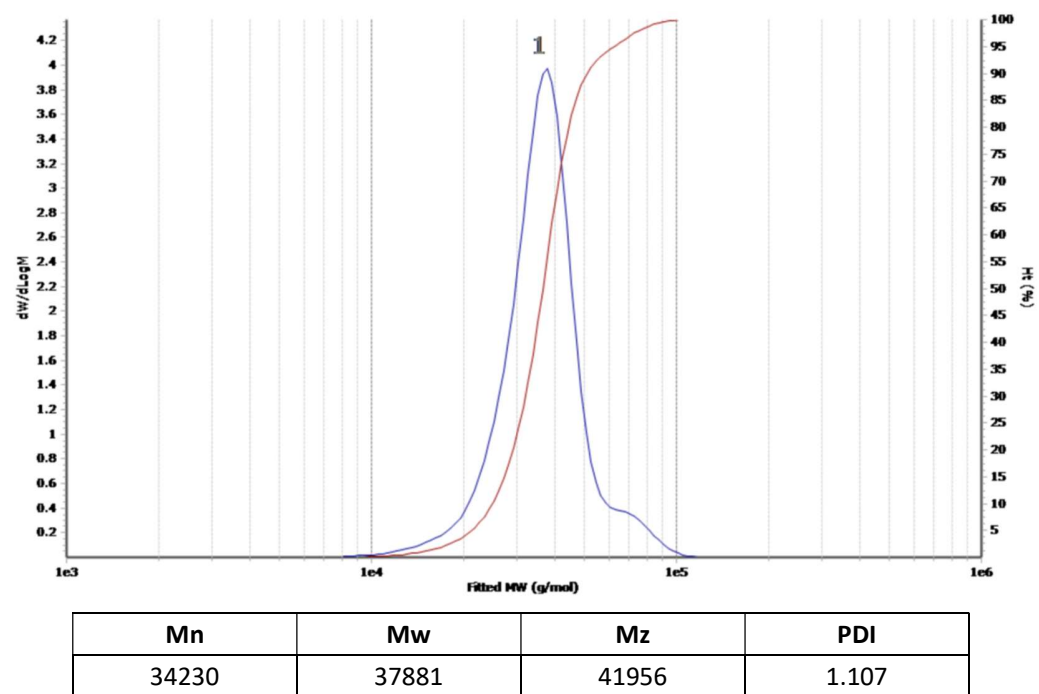


Figure S136. GPC curve and average molecular weight data of polybutadiene obtained by t-BuLi/**10** MeDiPz.

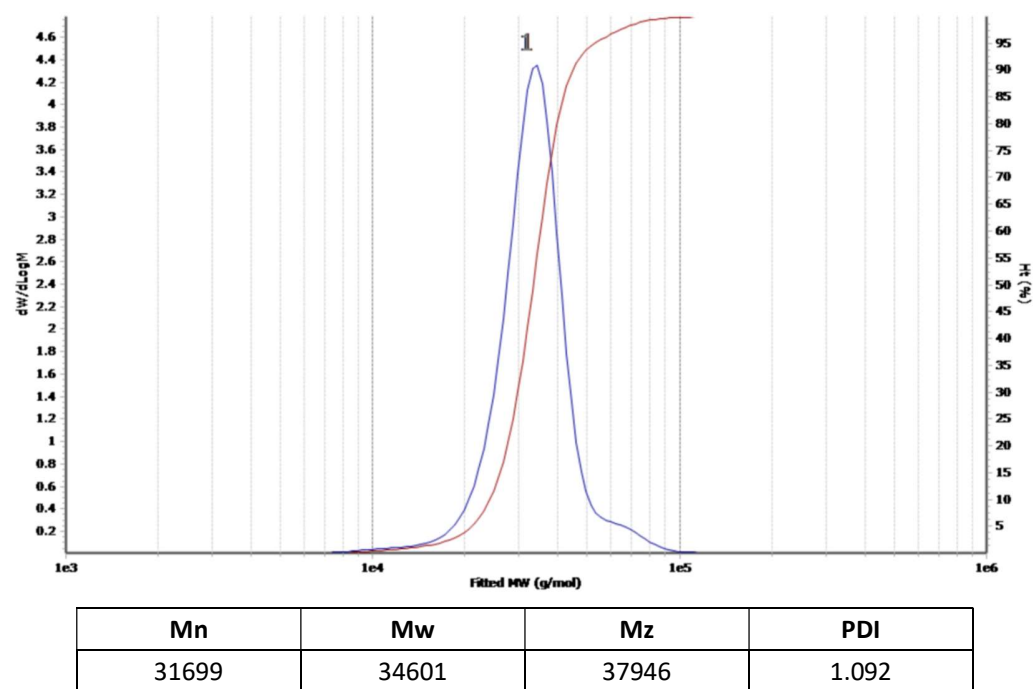


Figure S137. GPC curve and average molecular weight data of polybutadiene obtained by t-BuLi/**11** iPrDiPz.

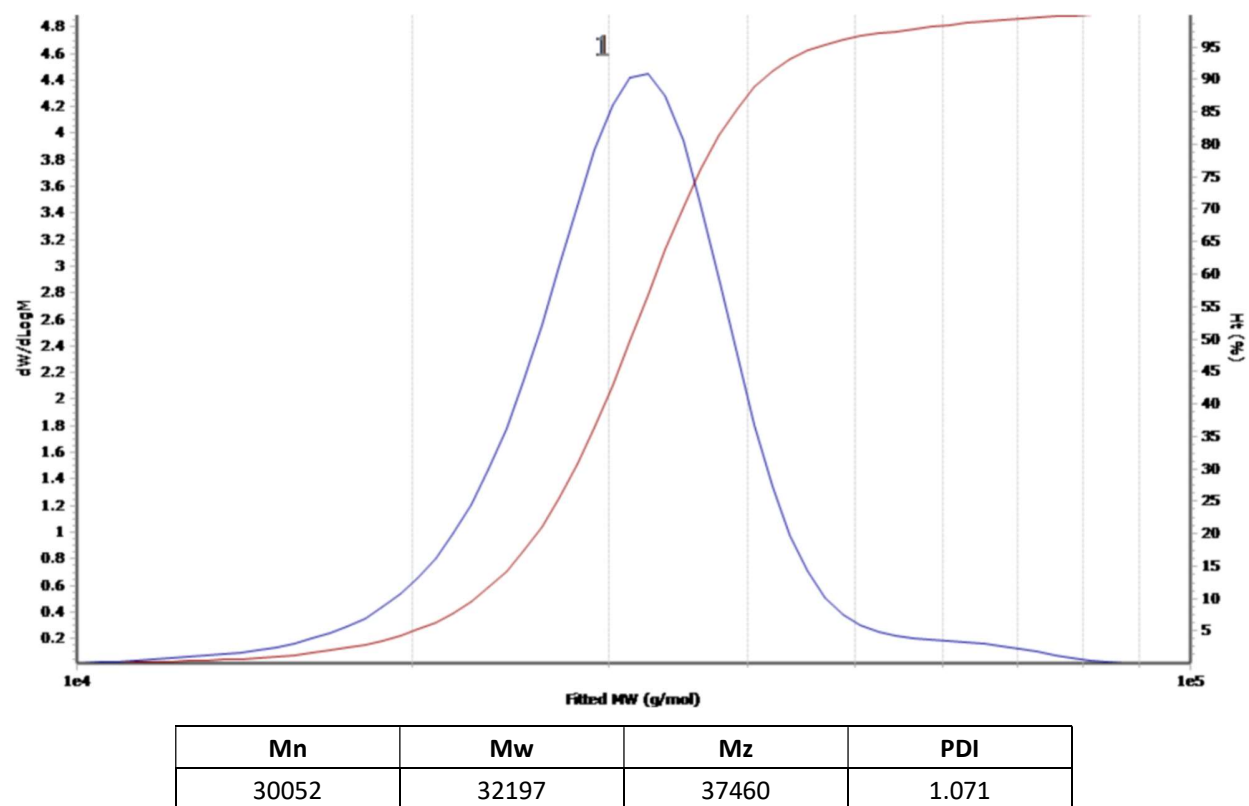


Figure S138. GPC curve and average molecular weight data of polybutadiene Initiated by **6a** complex, polymerization temperature 20°C.

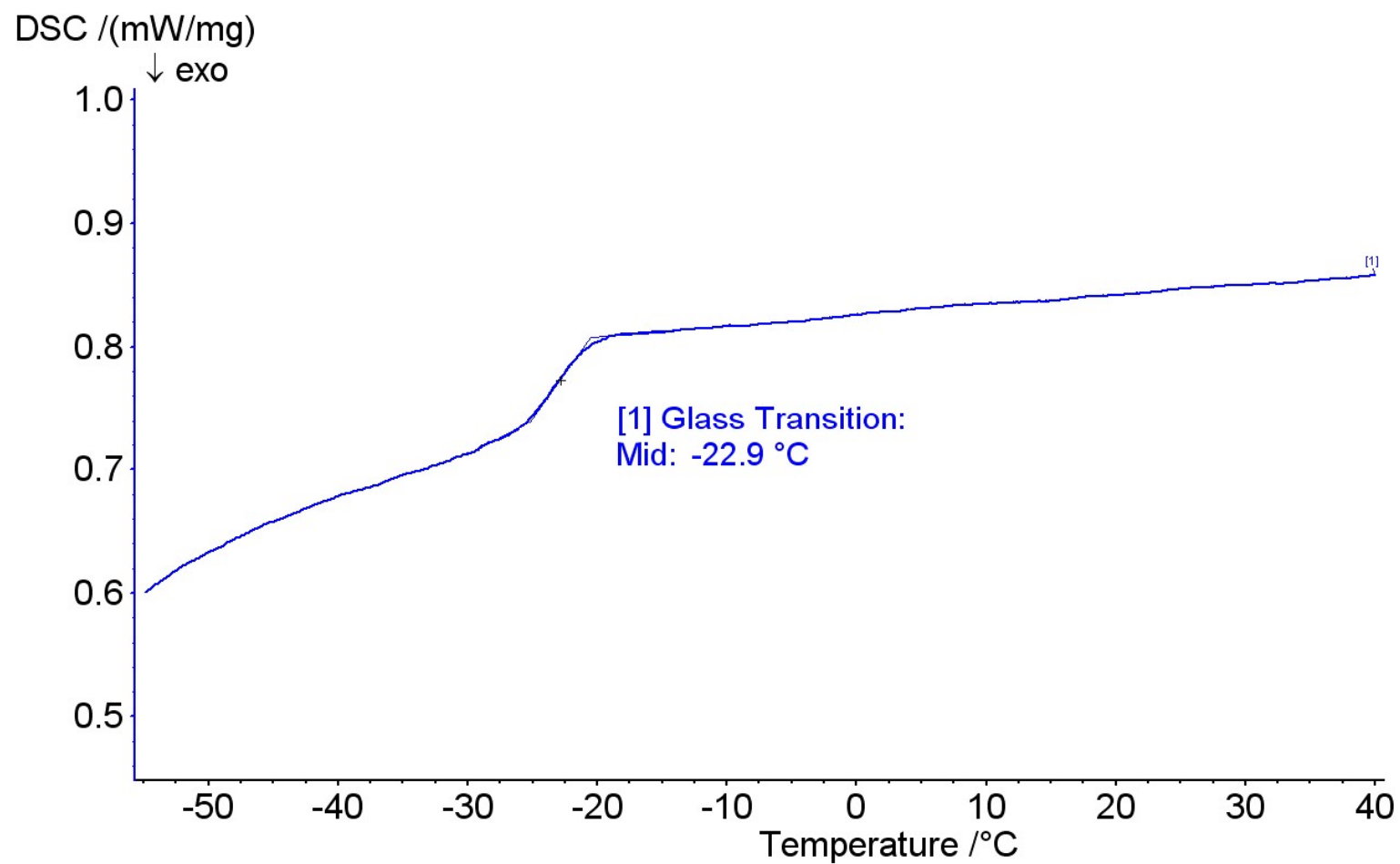


Figure S139. GPC curve of polybutadiene synthesized with Lewis base **3** TMEDA (polymerized at 0 °C)

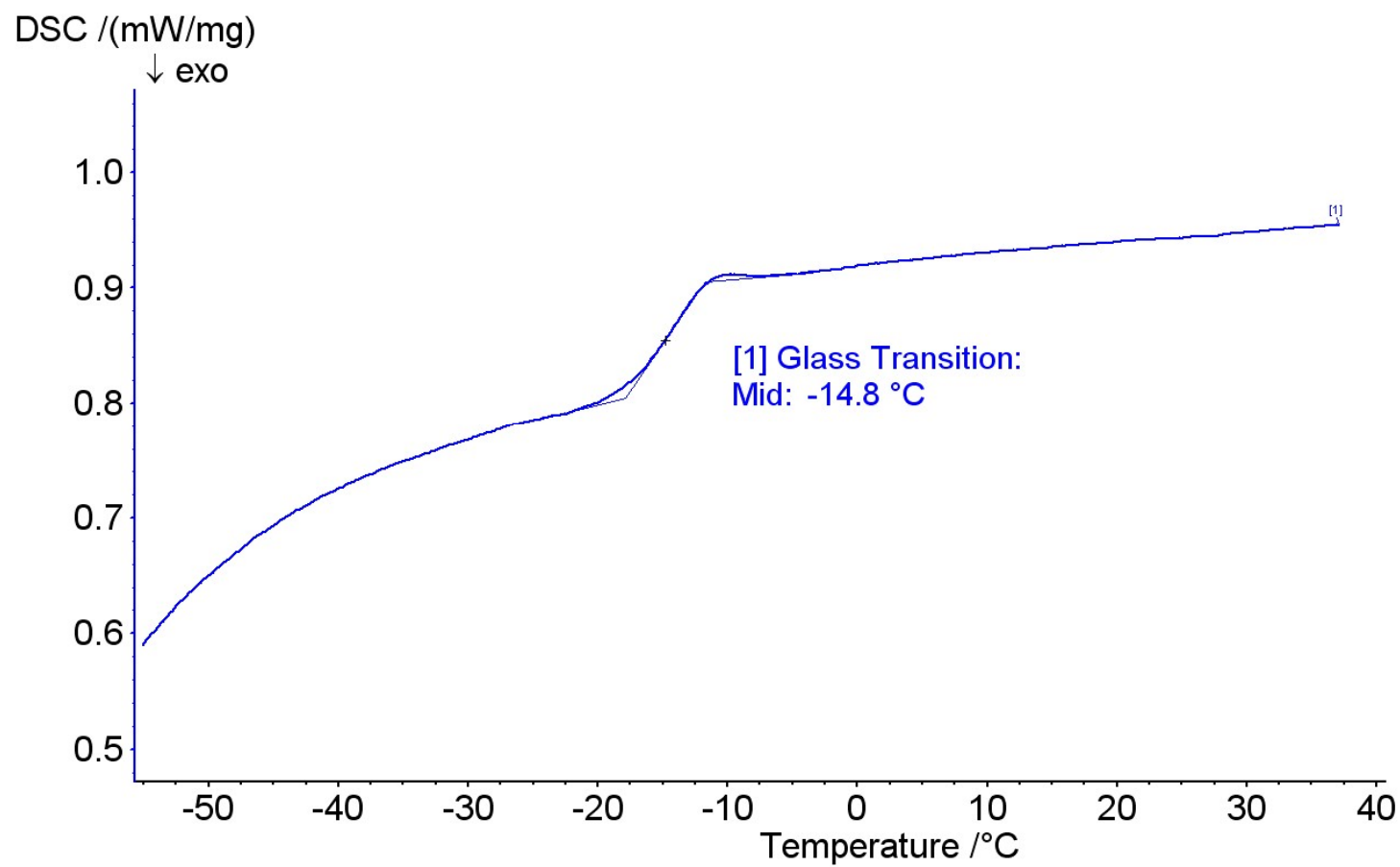


Figure S140. GPC curve of polybutadiene synthesized with Lewis base **4** TEEDA (polymerized at 0°C)

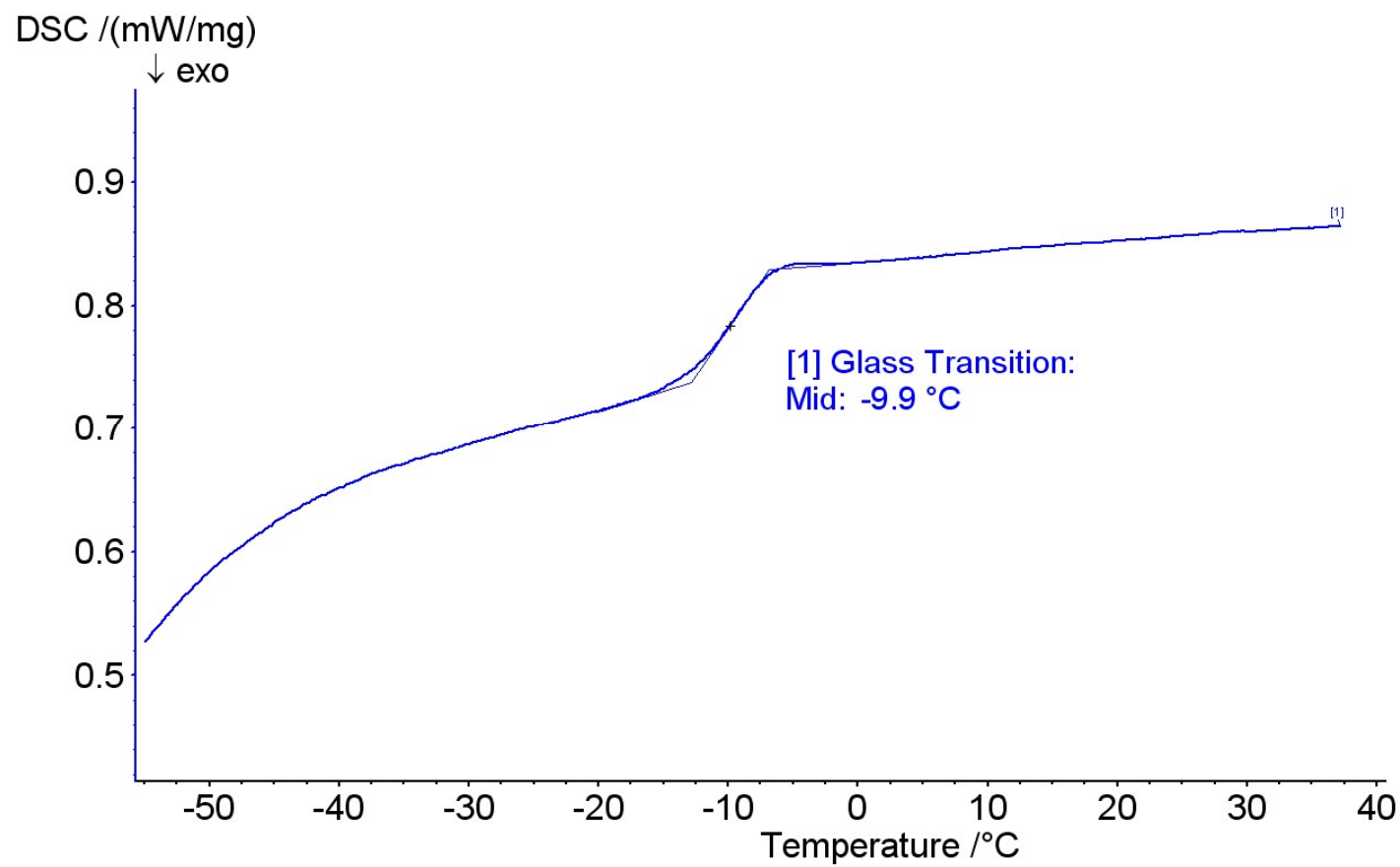


Figure S141. GPC curve of polybutadiene synthesized with Lewis base **5** DiPyr (polymerized at 0°C)

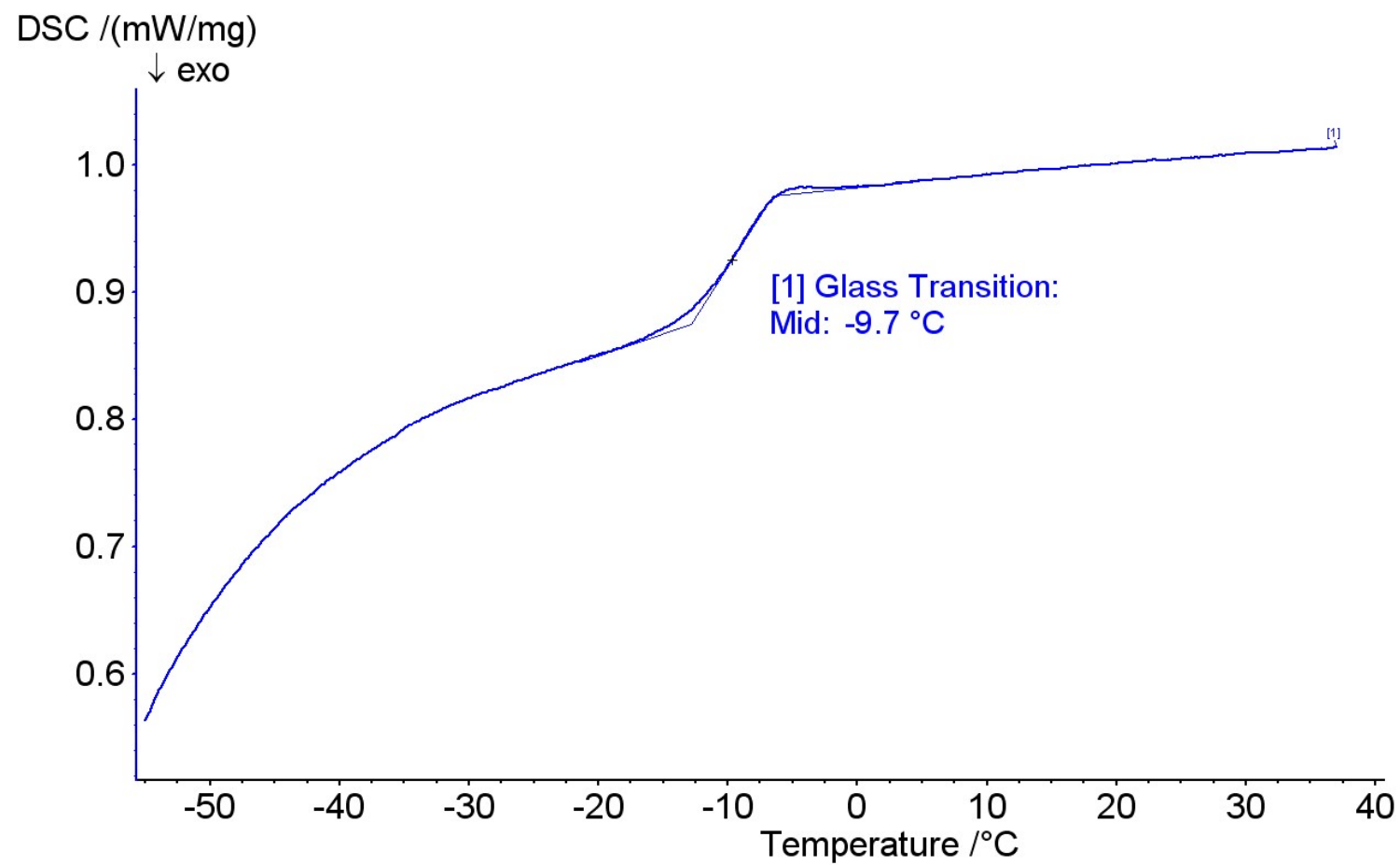


Figure S142. GPC curve of polybutadiene synthesized with Lewis base **6** DiPip (polymerized at 0°C)

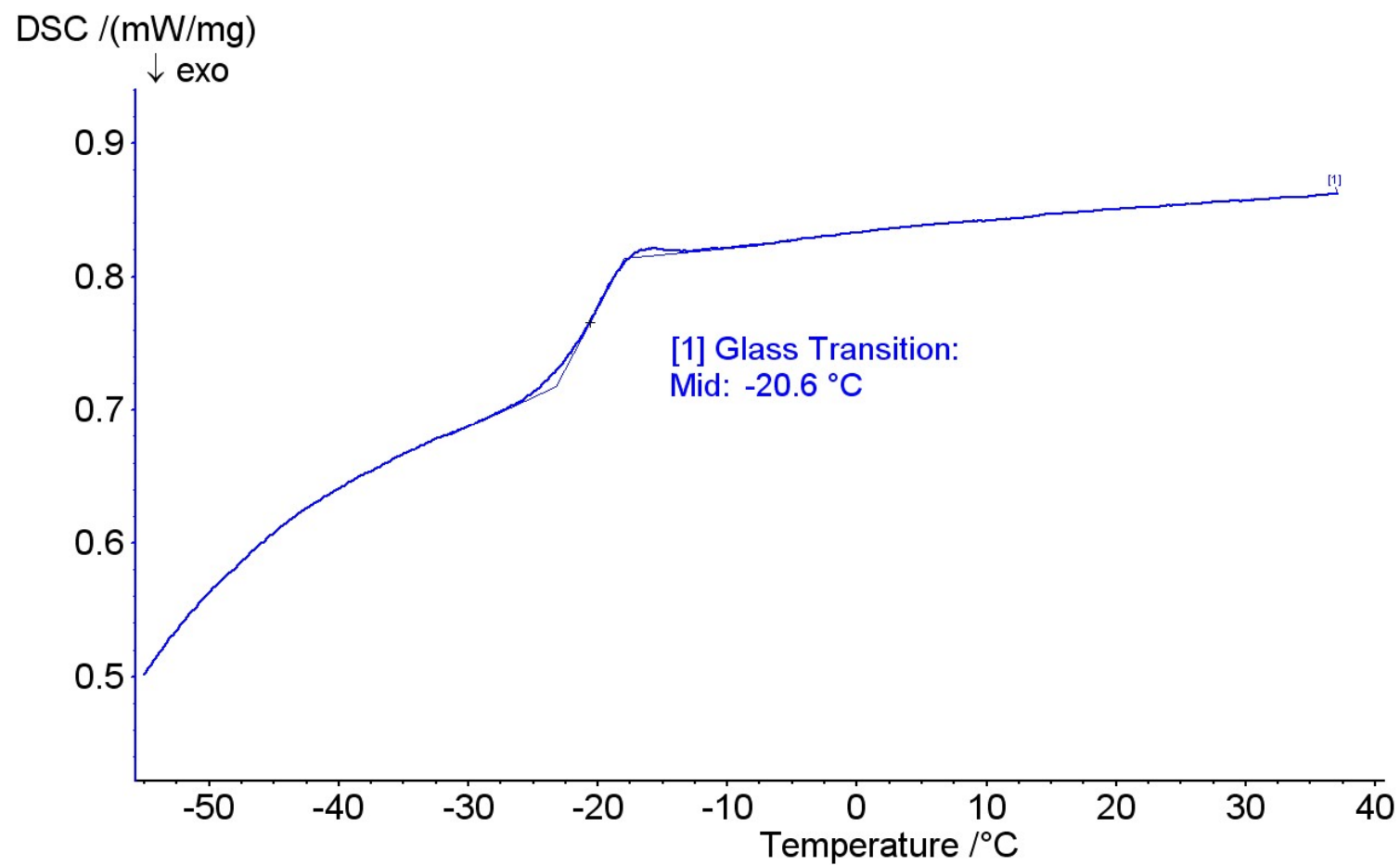


Figure S143. GPC curve of polybutadiene synthesized with Lewis base **7** DiAze (polymerized at 0°C)

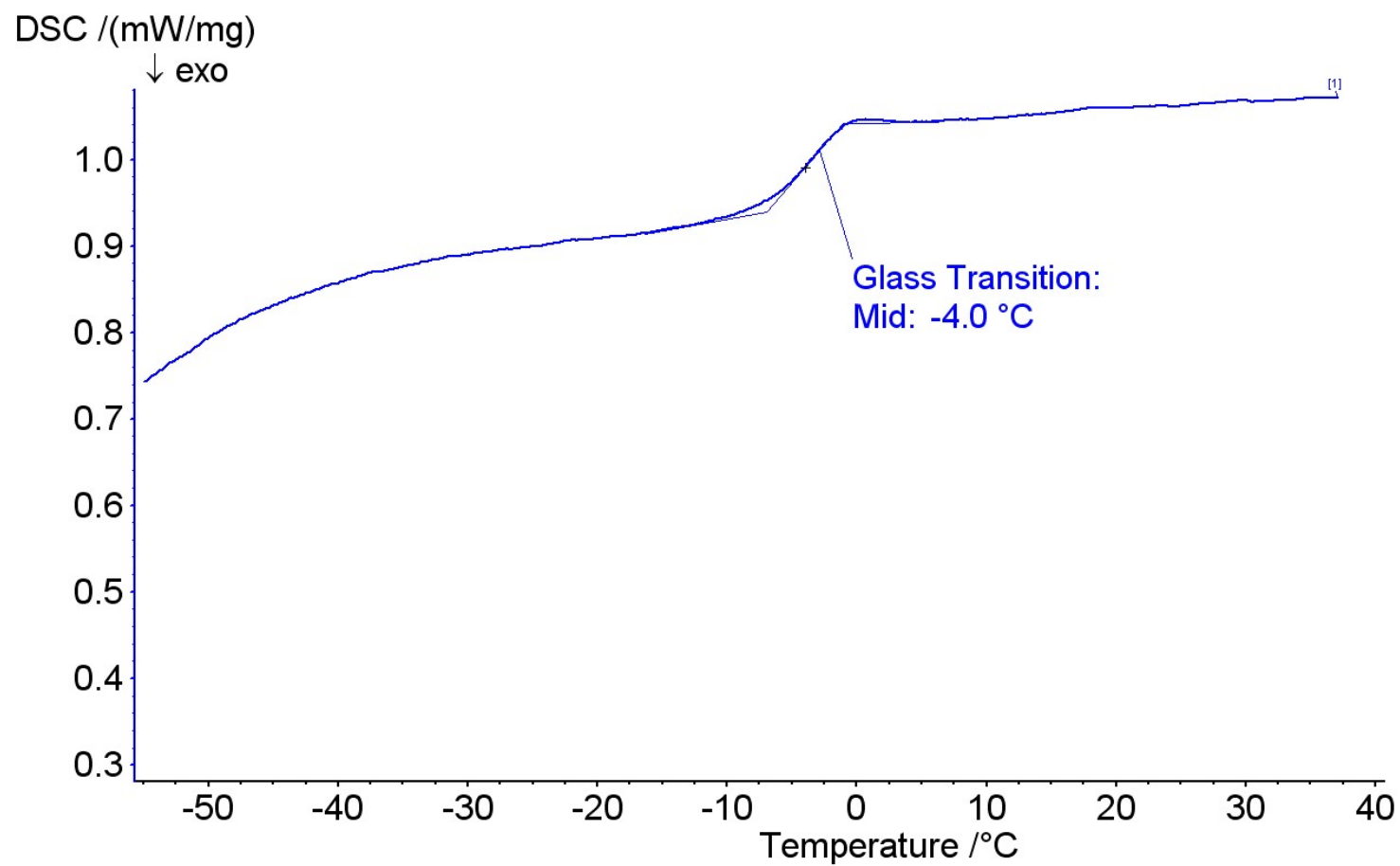


Figure S144. GPC curve of polybutadiene synthesized with Lewis base **8** MeDiPip (polymerized at 0°C)

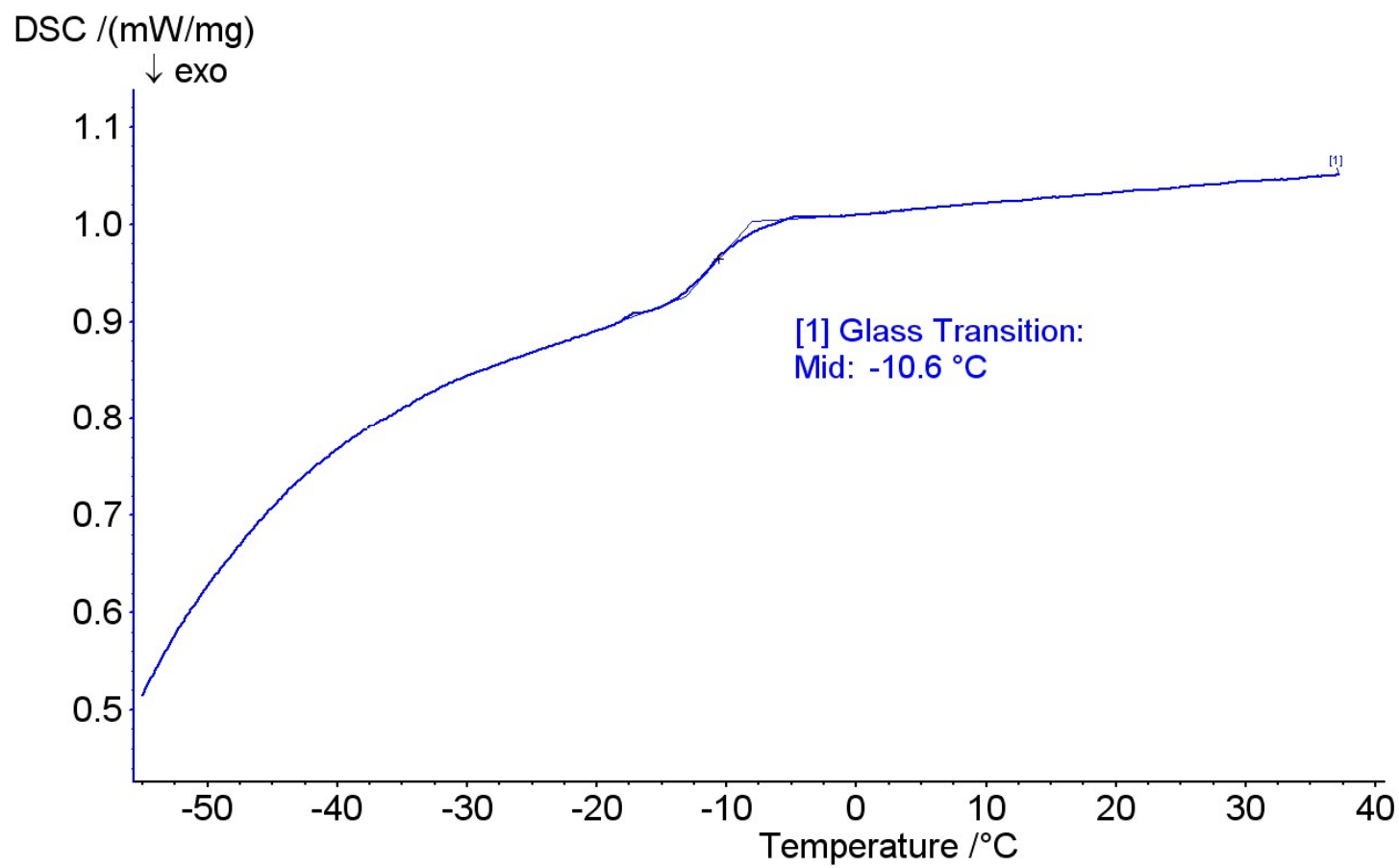


Figure S145. GPC curve of polybutadiene synthesized with Lewis base **9** DiMph (polymerized at 0°C)

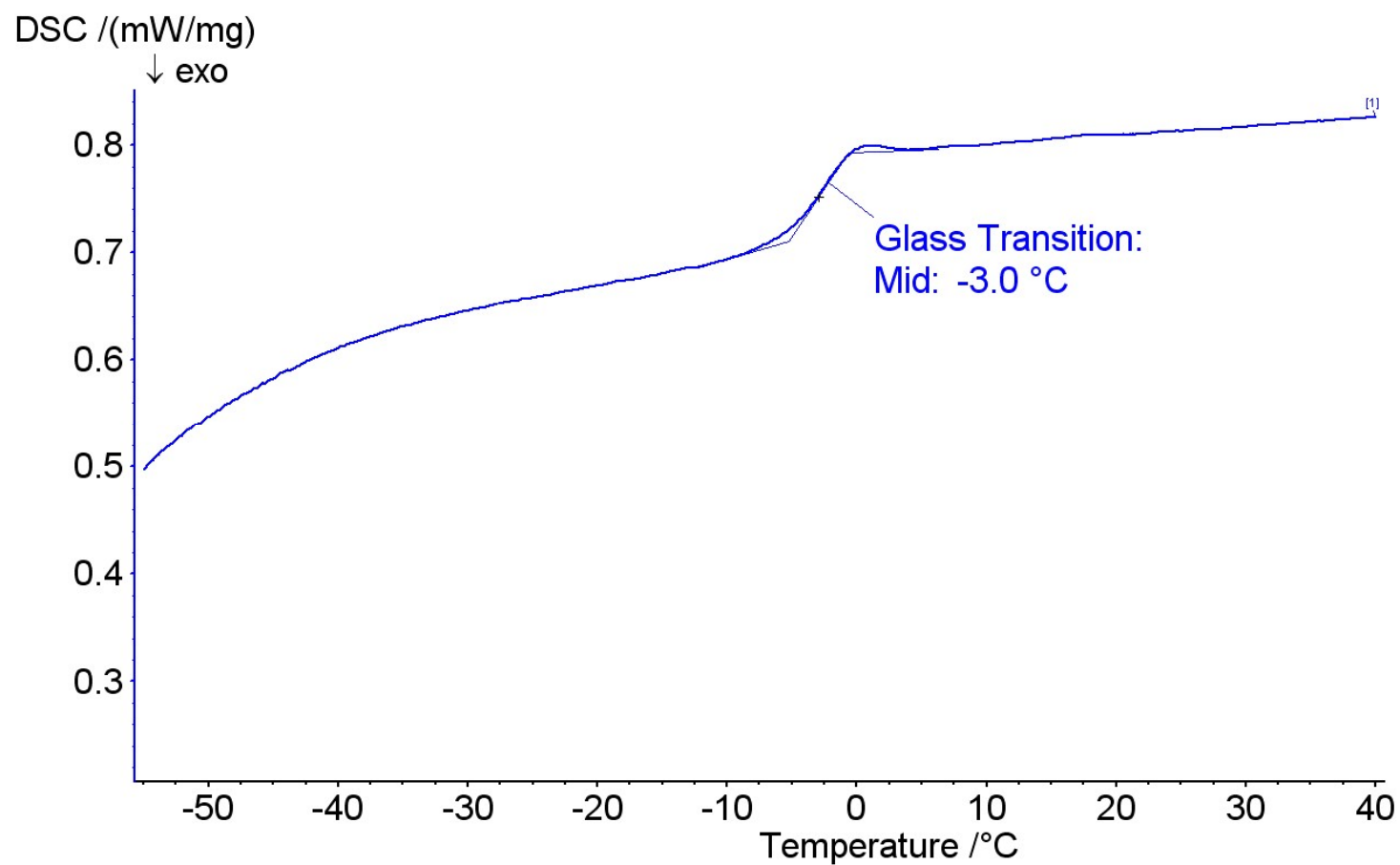


Figure S146. GPC curve of polybutadiene synthesized with Lewis base **10** MeDiPz (polymerized at 0°C)

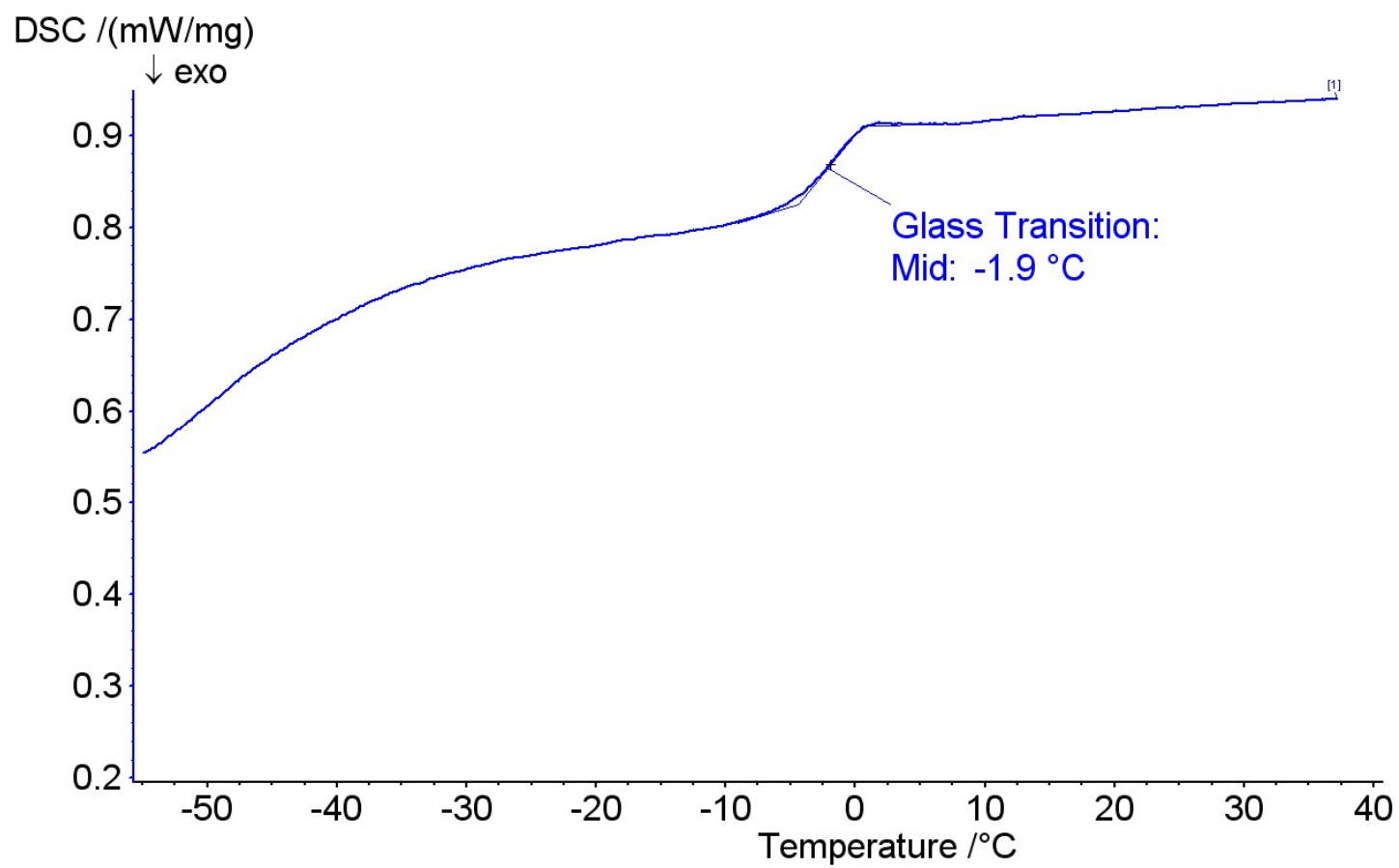


Figure S147. GPC curve of polybutadiene synthesized with Lewis base **11** iPrDiPz (polymerized at 0°C)

Energy Profile of Butadiene Anionic Polymerization with Various Lewis Bases as Ligand

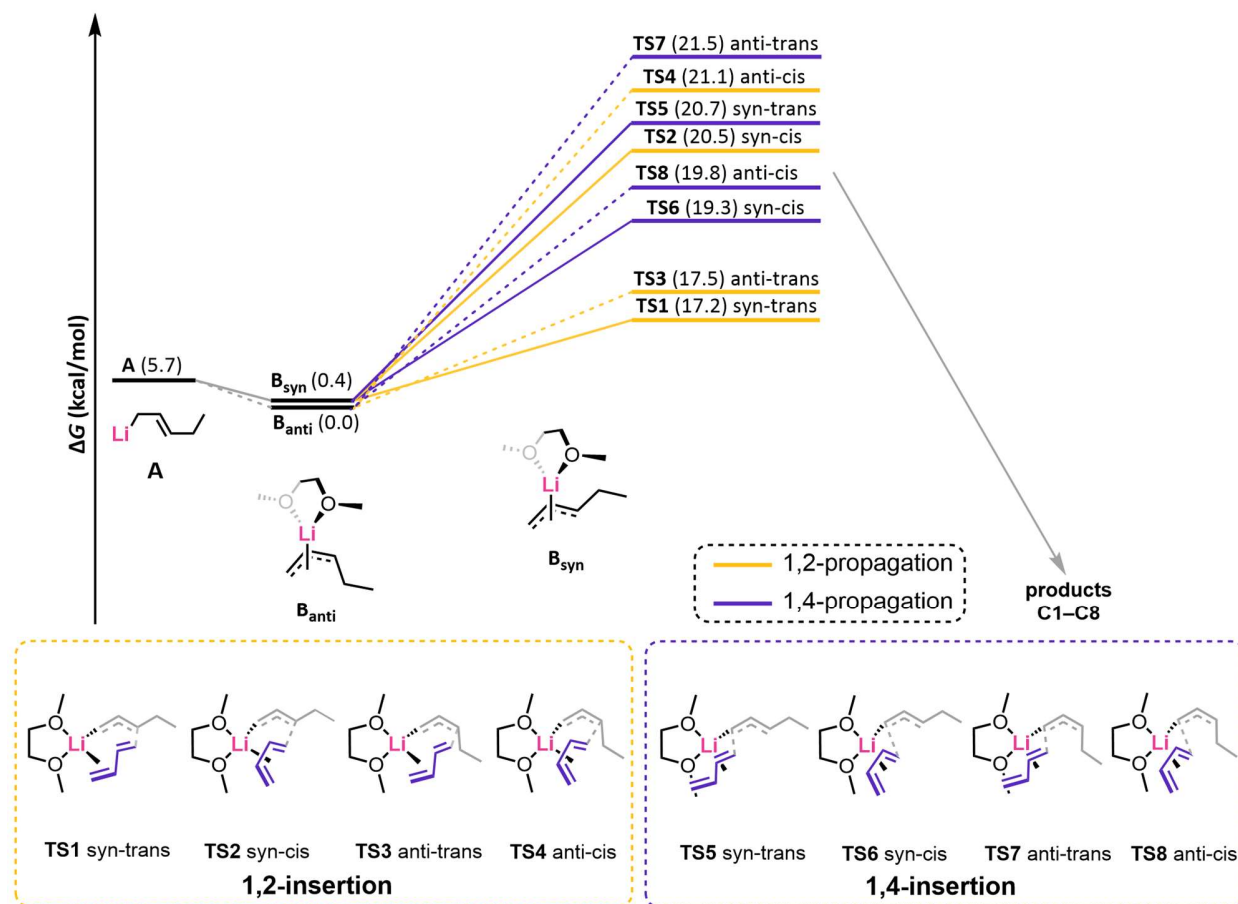


Figure S148. Energy profile of butadiene anionic polymerization with **1** glyme as ligand and potential transition states.

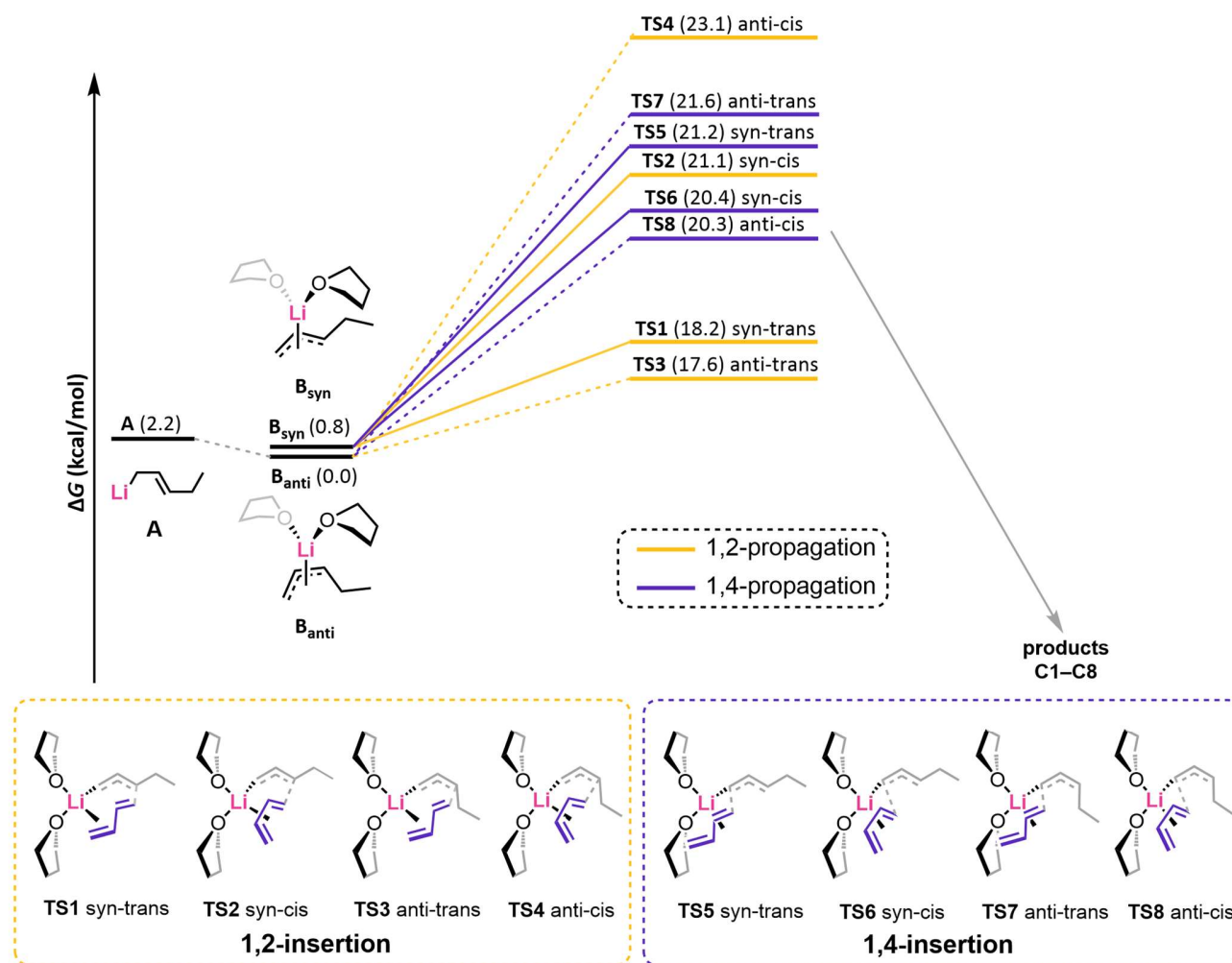


Figure S149. Energy profile of butadiene anionic polymerization with **2** THF as ligand and potential transition states.

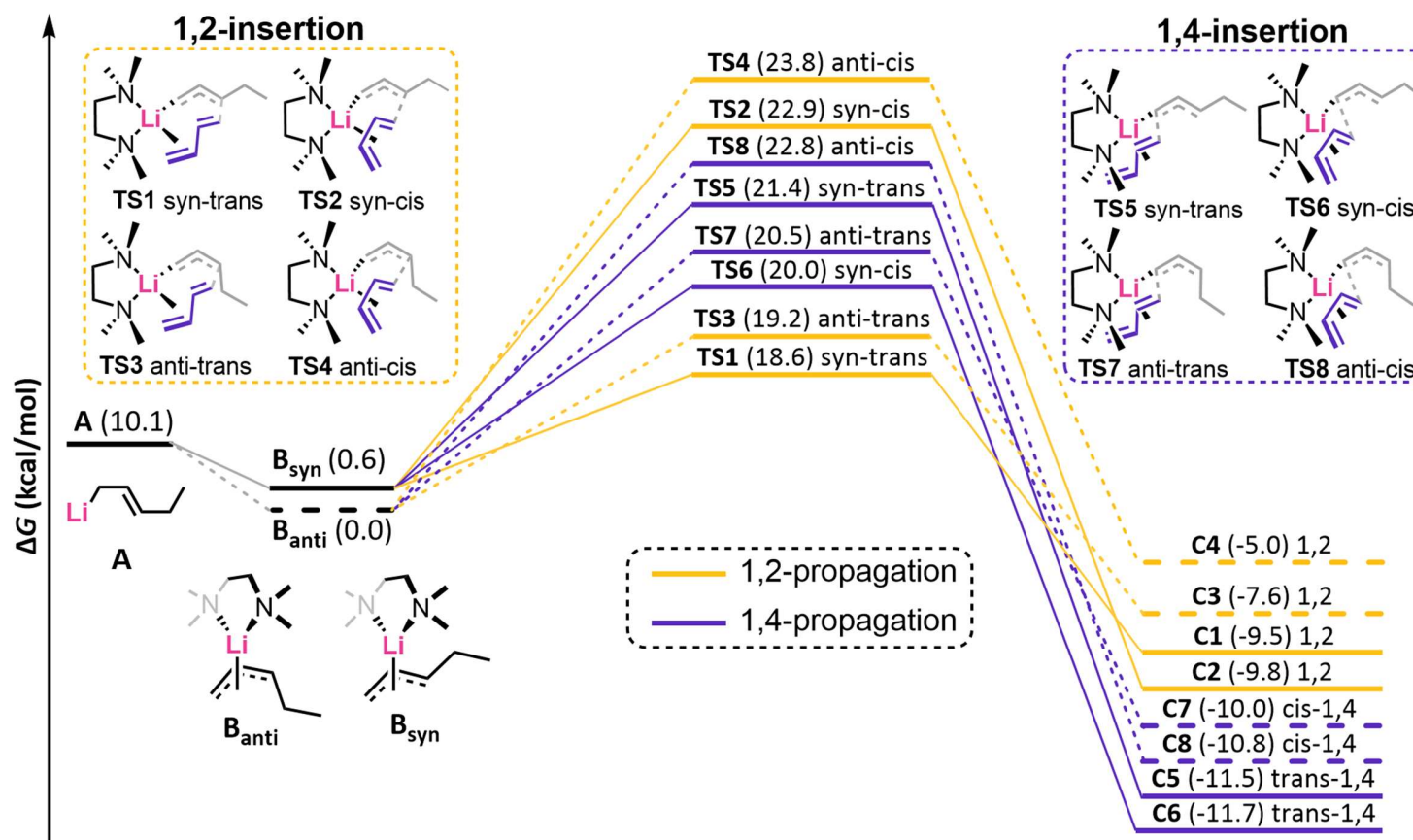


Figure S150. Energy profile of butadiene anionic polymerization with **3** TMEDA as ligand and potential transition states.

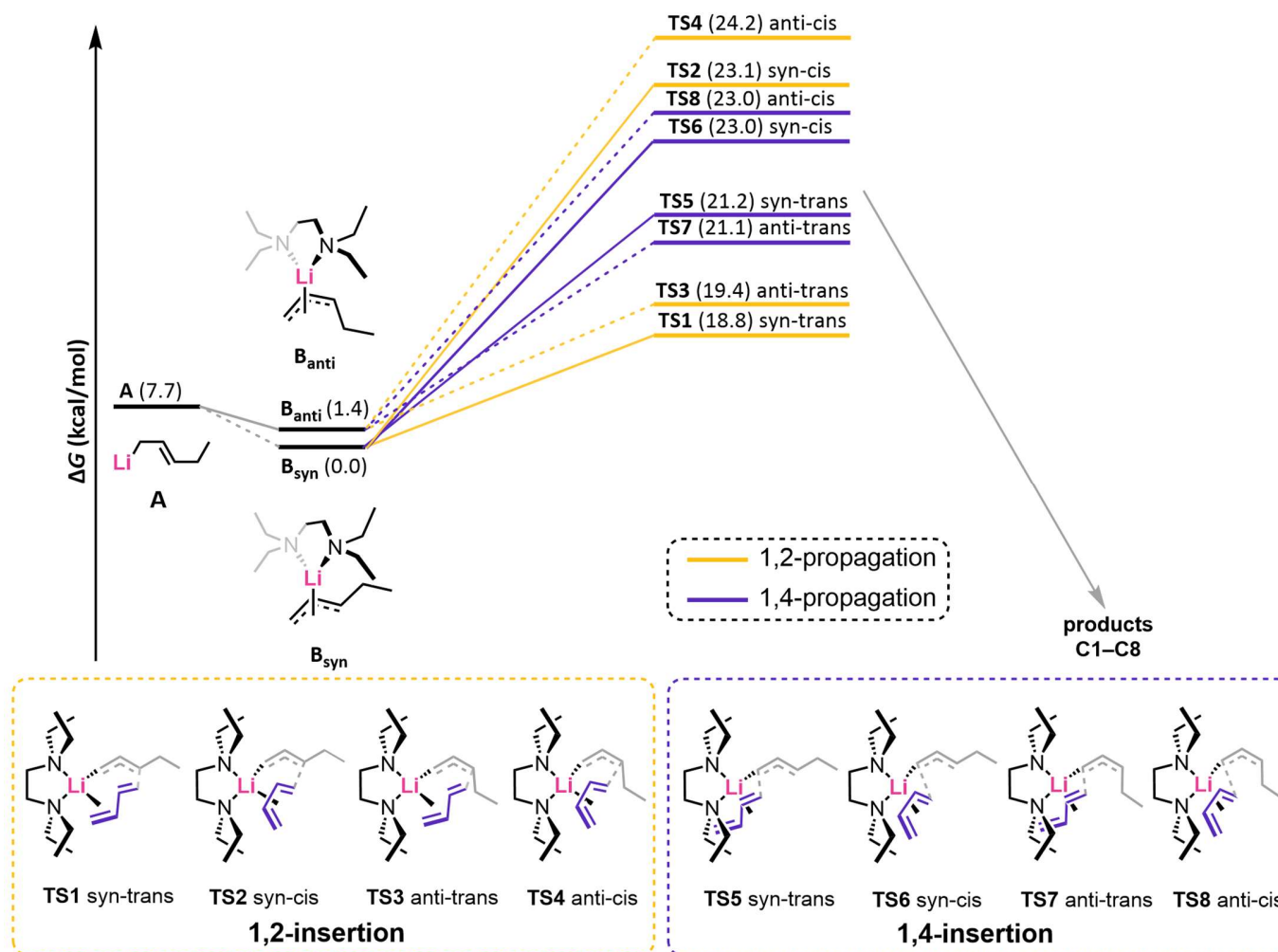


Figure S151. Energy profile of butadiene anionic polymerization with **4** TEEDA as ligand and potential transition states.

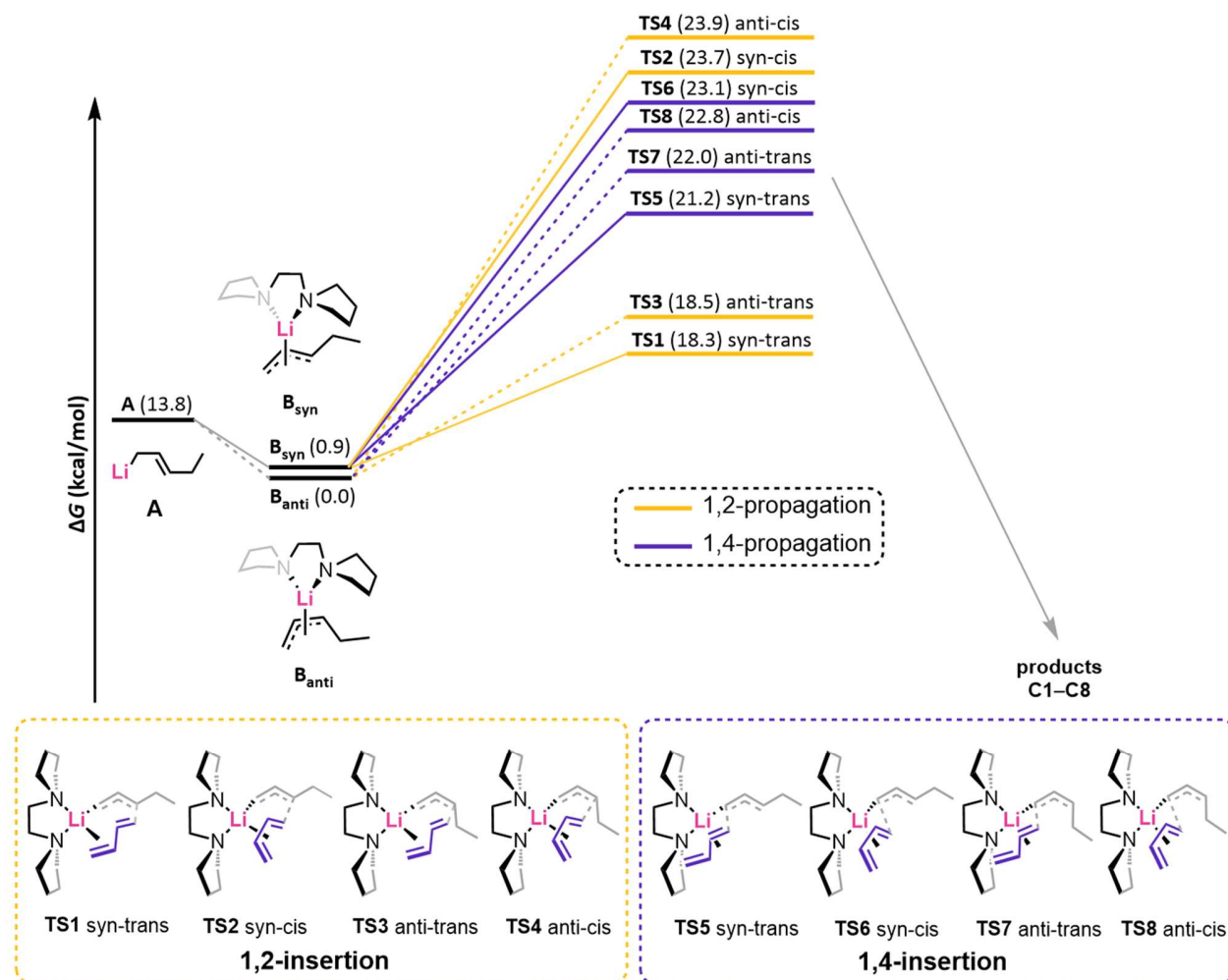


Figure S152. Energy profile of butadiene anionic polymerization with **5** DiPyr as ligand and potential transition states.

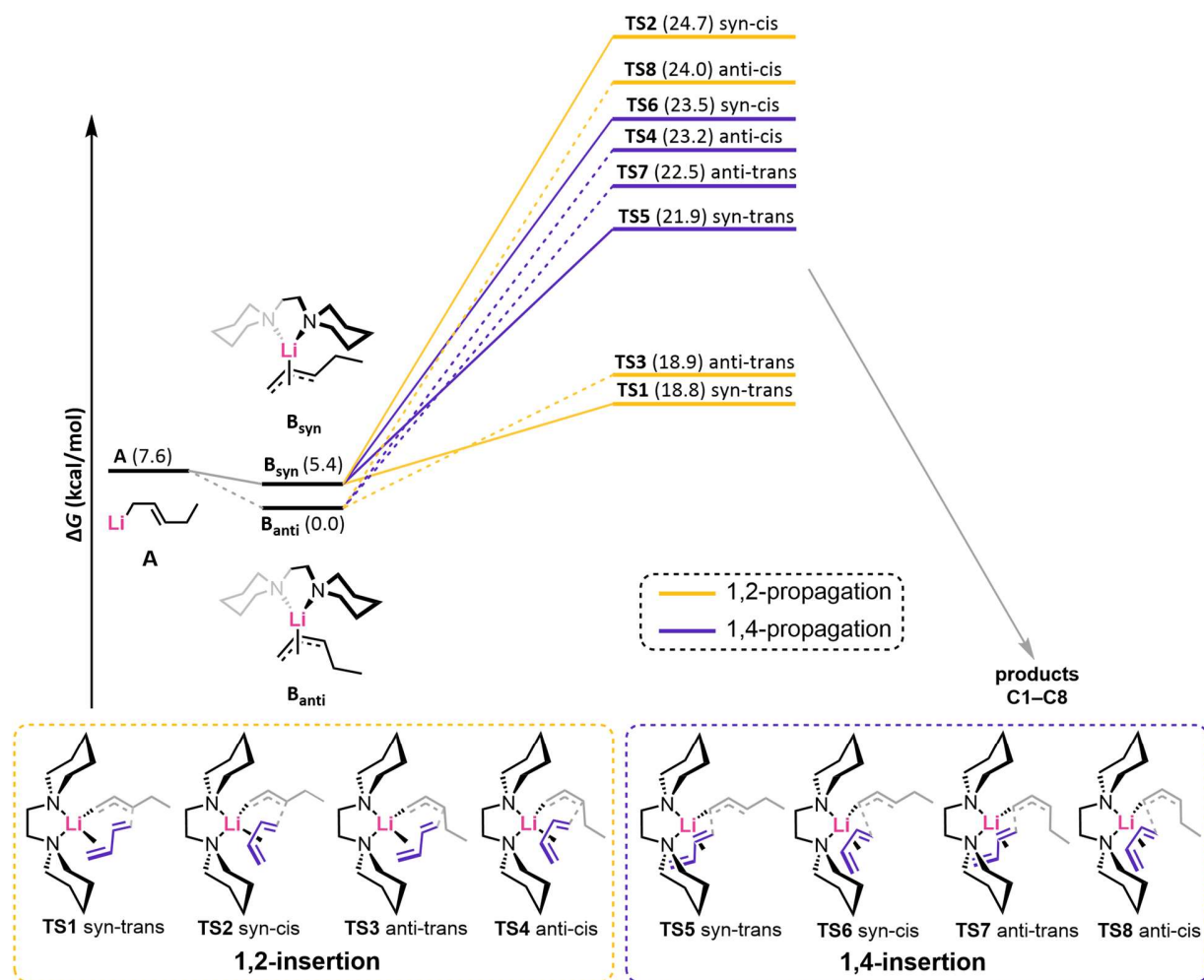


Figure S153. Energy profile of butadiene anionic polymerization with **6** DiPip as ligand and potential transition states.

Cartesian Coordinates of All Optimized Structures

1,3-Butadiene

C	-0.60786500	-0.40179400	-0.00000800
C	-1.84961000	0.10942000	0.00002700
H	-0.47345300	-1.48329000	-0.00001900
H	-2.01889000	1.18352700	0.00004600
H	-2.72873300	-0.52626500	0.00004200
C	0.60786500	0.40179400	-0.00002000
C	1.84961000	-0.10942000	-0.00000200
H	0.47345300	1.48329000	-0.00005500
H	2.72873300	0.52626400	-0.00002000
H	2.01889000	-1.18352700	0.00002800

3-Ethylallyllithium aggregate, a model of polybutadienyllithium

C	-4.42426000	-0.49652500	0.68598000
C	-3.29744700	-0.72830500	-0.34013600
C	-2.79312500	0.54964700	-0.97944400
C	-1.93358400	1.41444300	-0.34265000
C	-1.17005900	1.16577700	0.85679800
Li	-0.82421900	-0.34921600	-0.78454800
C	4.42714100	0.49316400	-0.68215900
C	3.29893000	0.72679700	0.34198800
C	2.79063200	-0.55041200	0.97964900
C	1.93063900	-1.41313100	0.34061600
C	1.17005700	-1.16226600	-0.86018400
Li	0.82449900	0.35295900	0.78109800
H	-4.74468900	-1.43669800	1.14998500
H	-4.09248200	0.18487900	1.47470200
H	-5.29104800	-0.04166500	0.19623400
H	-3.65272500	-1.41838500	-1.11481700
H	-2.48745000	-1.26586100	0.19267900
H	-3.25965900	0.85929100	-1.91006500
H	-1.69344300	2.33200300	-0.88329300
H	-0.75219000	2.07346800	1.30191200
H	-1.66059500	0.55269100	1.61825500
H	4.75043800	1.43289800	-1.14506300
H	5.29203100	0.03619500	-0.19102900
H	4.09539100	-0.18711600	-1.47186000

H	2.49113000	1.26648000	-0.19205700
H	3.65425800	1.41569400	1.11770300
H	3.25452200	-0.86147700	1.91111000
H	1.68761300	-2.33052200	0.88026300
H	0.75144700	-2.06884300	-1.30688300
H	1.66307100	-0.54939000	-1.62018100

TMEDA

C	0.59355700	0.48378000	-0.09959600
C	-0.59355700	-0.48378800	-0.09955400
N	-1.87248000	0.19709500	-0.30310600
N	1.87247900	-0.19712000	-0.30309600
C	-2.93188400	-0.76415400	-0.58150800
C	-2.23510000	1.05032600	0.82281000
C	2.93188300	0.76410600	-0.58158000
C	2.23510200	-1.05025800	0.82288900
H	0.44540400	1.18276000	-0.92914300
H	0.61502500	1.08029900	0.83418600
H	-0.61502300	-1.08022900	0.83427800
H	-0.44540700	-1.18283700	-0.92904300
H	-3.86607600	-0.23285900	-0.78775500
H	-2.67256900	-1.35595600	-1.46433200
H	-3.11223000	-1.46111100	0.26148600
H	-3.19530400	1.53326600	0.61893700
H	-1.48949200	1.83547600	0.96632600
H	-2.32769300	0.48369300	1.77151500
H	3.86607300	0.23279500	-0.78778600
H	2.67256500	1.35583600	-1.46445100
H	3.11223100	1.46113200	0.26135800
H	3.19530700	-1.53321300	0.61905400
H	1.48949600	-1.83539900	0.96647000
H	2.32769500	-0.48354800	1.77154800

TMEDA 3-ethylallyllithium complex (anti-isomer)

C	2.02569300	-1.04298200	-0.73441100
C	1.64805500	-1.71407500	0.43171200
C	1.43038800	-1.17211600	1.70991600
Li	0.15900000	-0.27867200	0.15721500
C	-2.08213500	1.36852400	-0.37108800

C	-2.61913900	0.03131000	0.13854600
N	-1.72379600	-1.08234200	-0.20763900
N	-0.71821600	1.64456200	0.11715700
C	-1.98670800	-2.25786300	0.62976100
C	-1.80749700	-1.44088500	-1.62849400
C	-0.72344300	2.06821100	1.52586400
C	-0.07351400	2.66958500	-0.71300700
H	1.30601700	-2.74291400	0.28797300
H	1.11015500	-1.82282400	2.51733400
H	1.93665000	-0.25954600	2.02026300
H	-2.77921900	2.17513400	-0.08455800
H	-2.04595400	1.35803500	-1.46414100
H	-2.70690400	0.05862800	1.22857100
H	-3.63752400	-0.12542800	-0.25951600
H	-1.83853900	-1.99776200	1.68007100
H	-3.01003800	-2.64671200	0.48866500
H	-1.27359100	-3.04535500	0.37650600
H	-2.81659000	-1.79515600	-1.90363400
H	-1.08098800	-2.22787400	-1.84051500
H	-1.55423800	-0.58434900	-2.25641400
H	-1.14565100	1.28518800	2.15812000
H	-1.30088500	2.99827400	1.66845800
H	0.30446600	2.23326000	1.85532700
H	0.93953500	2.85027700	-0.34814700
H	-0.62866900	3.62283000	-0.69702400
H	-0.00415700	2.31697200	-1.74515800
C	2.70451500	0.30770800	-0.68873200
C	4.18523400	0.25080500	-0.26054500
H	2.18819300	0.97959800	0.01942900
H	2.63433400	0.79961600	-1.66867000
H	4.63253700	1.25218500	-0.19601400
H	4.27797600	-0.23369800	0.71643600
H	4.76603100	-0.33747100	-0.97927300
H	2.13543800	-1.61975600	-1.64949900

TMEDA 3-ethylallyllithium complex (syn-isomer)

C	-2.06124200	-0.45145100	0.14056400
C	-1.84978700	-0.07584500	1.46639300
C	-0.99452400	-0.66508000	2.41542400
Li	0.05455700	-0.14156400	0.62740700

C	2.19885300	-0.36580600	-1.13374000
C	2.35610900	1.00385300	-0.46981200
N	1.06181700	1.54443300	-0.02463700
N	1.51527500	-1.32875200	-0.25260300
C	1.23099100	2.57070700	1.00939000
C	0.27112000	2.07261200	-1.14452800
C	2.39781400	-1.81840000	0.81488800
C	0.97206000	-2.45600600	-1.01883400
C	-3.00272500	0.28198100	-0.78045900
C	-4.41716900	-0.32409800	-0.86172500
H	-1.81112900	-1.47790300	-0.14927900
H	-2.25126700	0.90695900	1.73944200
H	-0.94153900	-0.25588000	3.41845600
H	-0.73792200	-1.72292500	2.32529500
H	3.19110600	-0.73726400	-1.44445500
H	1.59922300	-0.26712300	-2.04314500
H	3.00051300	0.91579000	0.40967900
H	2.86484100	1.69060100	-1.16889900
H	1.76114700	2.14572900	1.86522700
H	1.78894500	3.44832600	0.63952200
H	0.24720700	2.90044600	1.35174400
H	0.77861000	2.92017100	-1.63747600
H	-0.70131500	2.40196100	-0.77422500
H	0.08609300	1.29151200	-1.88396600
H	2.75680800	-0.98759500	1.42517100
H	3.26785900	-2.36304200	0.40837100
H	1.83328800	-2.48553000	1.46946300
H	0.43053100	-3.12382600	-0.34431700
H	1.76358100	-3.03442900	-1.52531800
H	0.26724700	-2.08487300	-1.76663900
H	-3.08864900	1.32678500	-0.44571800
H	-2.59380200	0.33034400	-1.80313300
H	-5.06183200	0.23097800	-1.55680500
H	-4.37156700	-1.36548800	-1.20228300
H	-4.89028700	-0.32361000	0.12638300

TEEDA

C	-0.66468500	0.37897400	-1.18413700
C	0.66469000	-0.37941400	-1.18402800
N	1.46501100	-0.23171600	0.02721800

N	-1.46503600	0.23156500	0.02711900
C	2.68893000	-1.02619900	-0.06857600
C	1.66032000	1.15557500	0.46041000
C	-1.66045900	-1.15561700	0.46060200
C	-2.68882300	1.02623300	-0.06875300
H	-1.21029900	0.05871400	-2.09435100
H	-0.47554800	1.45123000	-1.31575100
H	0.47558500	-1.45170300	-1.31540500
H	1.21032500	-0.05934700	-2.09429600
H	3.35378300	-0.66921000	-0.88035100
H	2.38424300	-2.04092000	-0.35302200
H	2.13390600	1.13066300	1.44645200
H	0.66640500	1.58125400	0.61960300
H	-0.66658200	-1.58138000	0.61981900
H	-2.13397900	-1.13047000	1.44667100
H	-2.38398900	2.04080800	-0.35356000
H	-3.35383500	0.66908600	-0.88032400
C	-3.47760800	1.10045100	1.23737900
H	-4.28174100	1.83752600	1.14335900
H	-3.94031500	0.14389400	1.49862000
H	-2.82472900	1.40231800	2.06285800
C	-2.48377100	-2.05565500	-0.47552700
H	-2.55028700	-3.06637300	-0.05809900
H	-3.50538500	-1.68347100	-0.60754900
H	-2.02792400	-2.13663300	-1.46812400
C	2.48349600	2.05548800	-0.47596100
H	2.55006000	3.06627400	-0.05870600
H	3.50509600	1.68329400	-0.60806200
H	2.02751100	2.13630000	-1.46850900
C	3.47791400	-1.09977300	1.23747600
H	2.82521700	-1.40146900	2.06316300
H	4.28220600	-1.83669400	1.14362800
H	3.94043300	-0.14300100	1.49827100

TEEDA 3-ethylallyllithium complex (syn-isomer)

C	-2.41806200	-0.48781700	0.24562200
C	-2.10574600	-0.02908300	1.52722700
C	-1.11686800	-0.48825800	2.41287000
Li	-0.27136800	-0.04631200	0.48812500
H	-2.57136600	0.92465000	1.80049400

H	-0.99454200	-0.00633900	3.37664700
H	-0.76721800	-1.51984400	2.35592400
C	-3.55774800	0.07345800	-0.56814900
C	-4.86674100	-0.73186500	-0.45662600
H	-3.28681300	0.13985400	-1.63417000
H	-3.75737500	1.10603500	-0.24734400
H	-5.66610700	-0.30207800	-1.07550900
H	-4.71173400	-1.76855500	-0.77927900
H	-5.21033600	-0.76079200	0.58334400
H	-2.10571700	-1.49928000	-0.02954300
C	2.05521200	0.91953700	-0.75918000
C	1.71831500	-0.45156800	-1.34490200
N	1.12692500	-1.36714200	-0.35257600
N	0.86708900	1.57965600	-0.18499600
C	0.54758200	-2.53757900	-1.04971800
C	2.06077000	-1.73383600	0.73670400
C	0.11084300	2.28884300	-1.24231900
C	1.20540600	2.43221900	0.97658300
H	2.51957200	1.53226000	-1.54823100
H	2.80550900	0.81141000	0.02844300
H	0.98259500	-0.33381800	-2.14720800
H	2.62200500	-0.87397600	-1.81408600
H	1.30111500	-3.01497000	-1.69953800
H	-0.23454800	-2.14533800	-1.70833600
H	1.49095100	-2.31218400	1.46583800
H	2.33949000	-0.81445800	1.25824000
H	0.75807300	3.02584200	-1.74788300
H	-0.16123900	1.54247200	-1.99514100
H	0.26810500	2.73544900	1.44878800
H	1.70659100	1.78526400	1.70355300
C	2.07110200	3.66183000	0.68019000
H	2.28763200	4.19327800	1.61248200
H	3.02833700	3.38657600	0.22477600
H	1.56729100	4.36411700	0.00885000
C	-1.16128900	2.96347800	-0.74223000
H	-1.73914600	3.32756600	-1.59700100
H	-1.78028200	2.25142800	-0.19236200
H	-0.94942500	3.82116500	-0.09737600
C	3.32268700	-2.50259900	0.32737100
H	3.90879000	-2.74122900	1.22061300
H	3.08199100	-3.44605500	-0.17243300

H	3.96514400	-1.92160900	-0.34169900
C	-0.06035600	-3.58556900	-0.12197800
H	-0.75398100	-3.13311400	0.59096000
H	-0.61822300	-4.31245300	-0.72008200
H	0.70022200	-4.13707700	0.43811100

TEEDA 3-ethylallyllithium complex (anti-isomer)

C	1.61911400	-2.29073100	-0.61006800
C	1.03393600	-2.59910900	0.62059600
C	1.18478100	-1.92865200	1.84634700
Li	0.38887400	-0.64514700	0.23960600
C	-0.84371000	1.79296900	-0.45345900
C	-1.91054700	0.92570100	0.21409800
N	-1.68076200	-0.50157500	-0.03309400
N	0.51101200	1.46283800	0.01449500
C	-2.34384400	-1.37721600	0.95163900
C	-1.84158100	-0.91711100	-1.44530700
C	0.77666200	1.83902000	1.42681900
C	1.55572700	1.88245200	-0.94108400
H	0.22634900	-3.33544200	0.58015400
H	0.64049900	-2.28161000	2.71658100
H	2.08711900	-1.35807000	2.06018200
H	-1.10220800	2.85009400	-0.29757800
H	-0.86322100	1.62775100	-1.53525900
H	-1.88318000	1.07720600	1.29813300
H	-2.90002100	1.26971100	-0.12312700
H	-1.95431100	-1.08807800	1.93344400
H	-1.97863800	-2.39267600	0.77262700
H	-1.82328500	-2.01025500	-1.44833500
H	-0.94232800	-0.61271300	-1.99397100
H	0.32595000	1.07346700	2.06907500
H	1.85630300	1.73992700	1.57282700
H	2.50735700	1.49005200	-0.57267500
H	1.35004200	1.35258700	-1.87839700
C	2.88196500	-1.46480800	-0.70308200
C	4.16288700	-2.23639500	-0.32484500
H	2.82229800	-0.58895900	-0.03461100
H	2.99694600	-1.05738200	-1.71713600
H	5.05431700	-1.59524400	-0.36226300
H	4.07247400	-2.64532500	0.68640700

H	4.31718800	-3.07668700	-1.01058100
H	1.37270900	-2.91252700	-1.46750900
C	1.70003000	3.38237400	-1.23025800
H	2.42437100	3.52639300	-2.03906100
H	0.75434700	3.83250300	-1.54905700
H	2.06569200	3.93360400	-0.35997000
C	0.30834400	3.22032000	1.90462600
H	0.63379600	3.36338500	2.94027200
H	0.71804800	4.03806400	1.30763300
H	-0.78255700	3.30959500	1.89457700
C	-3.07381500	-0.40735000	-2.20618300
H	-3.07506400	-0.84054100	-3.21195100
H	-4.01233400	-0.68239900	-1.72008100
H	-3.06286300	0.68114500	-2.32307800
C	-3.87795600	-1.37611100	0.98442600
H	-4.30892700	-1.81813100	0.08194800
H	-4.22275800	-1.96936100	1.83820200
H	-4.28443900	-0.36559800	1.09835100

DiPyr

C	2.48450100	0.76303300	0.91748600
C	2.90889700	-1.17794500	-0.23784500
C	3.16908500	1.24111100	-0.39740500
H	3.23158100	0.65107900	1.71208000
H	1.72148600	1.45482400	1.28178200
C	3.39690400	-0.06603200	-1.20298100
H	2.49413500	-2.05287900	-0.74530300
H	3.74261300	-1.52064300	0.38821500
H	2.52605300	1.93444000	-0.94794200
H	4.10383400	1.76898700	-0.18616000
H	2.80130200	-0.06524600	-2.12152800
H	4.44217800	-0.20697700	-1.49395000
C	-0.50496300	-0.28502400	1.11529500
H	-0.23766300	0.57290800	1.74304000
H	-0.48603100	-1.16459700	1.76932300
C	-2.16671700	1.17424600	-0.03505300
C	-2.47077800	-1.12634700	-0.16407500
C	-3.63737400	1.00226900	-0.46578400
H	-1.53034200	1.32912100	-0.92770200
H	-2.00705300	2.02501700	0.63634100

C	-3.84763400	-0.53991100	-0.52632200
H	-2.52913900	-2.06462200	0.39831900
H	-1.89404600	-1.32497100	-1.08853400
H	-4.30741700	1.45141400	0.27228600
H	-3.83219400	1.48749800	-1.42652400
H	-4.59680600	-0.85188300	0.20645700
H	-4.18498600	-0.87873600	-1.51010700
N	-1.86933000	-0.07815000	0.65342000
N	1.90423300	-0.56238900	0.64078000
C	0.57042900	-0.47897500	0.02995500
H	0.49883600	0.32261300	-0.72587500
H	0.38522600	-1.42213000	-0.49324200

DiPyr 3-ethylallyllithium complex (syn-isomer)

C	0.76935000	2.02078800	0.10218100
C	1.01823800	1.58830700	1.40231700
C	0.10368800	1.10636400	2.35858800
Li	-0.06340000	0.00997100	0.52820800
C	-1.33420500	-1.42219700	-1.46742300
C	-0.39515200	-2.43222100	-0.80957100
C	1.84540200	2.53488000	-0.81927400
C	1.96046800	4.07075100	-0.86382200
H	-0.25248700	2.31792700	-0.15423400
H	2.07617600	1.43475700	1.64254300
H	0.46289600	0.81207300	3.33883000
H	-0.93465600	1.43834700	2.32254000
H	-2.17042100	-1.95712300	-1.95239900
H	-0.79905000	-0.87747000	-2.25229800
H	-0.93471700	-2.97953100	-0.03010500
H	-0.06837800	-3.17507600	-1.55836100
H	2.81515900	2.12234600	-0.50561600
H	1.68816600	2.17655500	-1.85037800
H	2.74208600	4.40256500	-1.56051900
H	1.01223000	4.52006800	-1.18252300
H	2.19164200	4.46541100	0.13163400
C	1.45677100	-2.60721100	0.79903300
C	1.80180900	-1.34992900	-1.14180400
C	2.73485500	-1.81505600	1.08173800
H	1.69243600	-3.59683000	0.36646300
H	0.83026900	-2.75552100	1.68321700

C	3.05630100	-1.12451000	-0.27120900
H	1.49625300	-0.44860600	-1.67860100
H	1.97496300	-2.15345000	-1.87938300
H	2.53291000	-1.06497100	1.85080200
H	3.54593800	-2.45662900	1.43558200
H	3.24457800	-0.05930000	-0.12955300
H	3.93778200	-1.55660300	-0.75249400
C	-2.52152300	0.69692800	-1.13033900
C	-2.81786600	-0.98242000	0.45818100
C	-3.20900800	1.40259300	0.04425600
H	-3.26791800	0.33169700	-1.85874800
H	-1.80141900	1.32577000	-1.66058200
C	-3.49052900	0.26436200	1.06406100
H	-2.32974000	-1.60619400	1.21113200
H	-3.55544000	-1.60573400	-0.07902700
H	-2.53674800	2.14574900	0.48084300
H	-4.11733600	1.92106400	-0.27293000
H	-3.05485600	0.50109600	2.03698600
H	-4.56028800	0.09425600	1.21118800
N	0.75080700	-1.76740600	-0.18539700
N	-1.82815300	-0.44047100	-0.49747500

DiPyr 3-ethylallyllithium complex (anti-isomer)

C	-0.25956100	2.36710200	-0.55239500
C	0.25641900	2.33072500	0.74416700
C	-0.27565900	1.69683400	1.88139700
Li	0.09600100	0.29489500	0.23219000
C	0.12807500	-2.31901000	-0.78609000
C	1.42245200	-2.15759000	0.00445300
C	-1.72162900	2.11361900	-0.83896500
C	-2.64569800	3.29438900	-0.47795400
H	0.30356600	2.90264800	-1.31335300
H	1.28392300	2.68752600	0.84443400
H	0.26609000	1.75231500	2.82023600
H	-1.34866700	1.54006800	1.97479700
H	-0.15614800	-3.38640000	-0.81008900
H	0.28826200	-2.00716000	-1.82339600
H	1.25635900	-2.45132900	1.04578400
H	2.18955600	-2.83968100	-0.40408700
H	-1.86266500	1.86238900	-1.89961700

H	-2.07618600	1.23803800	-0.27472900
H	-3.70316500	3.05833300	-0.66070300
H	-2.52714300	3.55778300	0.57782200
H	-2.38610400	4.17763800	-1.07162400
C	2.93257600	-0.52199800	1.01571000
C	2.52071500	-0.36156900	-1.27909600
C	3.61777400	0.78442400	0.57601400
H	3.65810500	-1.35446900	1.02237800
H	2.46962900	-0.45954600	2.00402800
C	3.25594900	0.93724600	-0.92677500
H	1.76654900	-0.22071200	-2.05776300
H	3.22922100	-1.13993800	-1.61783200
H	3.24078300	1.63202400	1.15162800
H	4.69753400	0.72915300	0.73815700
H	2.58555100	1.78642300	-1.07309900
H	4.13429700	1.08346100	-1.56088300
C	-2.13434400	-1.47782300	-1.14076700
C	-1.48439500	-2.01142900	1.05475700
C	-3.35844200	-1.18794400	-0.24364100
H	-2.24613800	-2.45788700	-1.63263900
H	-1.97852700	-0.72605000	-1.91904000
C	-2.82144800	-1.28628100	1.20489300
H	-0.79122100	-1.78886200	1.87011300
H	-1.62971200	-3.10634500	1.00449000
H	-3.78274600	-0.20195800	-0.44508100
H	-4.14429400	-1.92576400	-0.42815200
H	-2.64616200	-0.29039300	1.61917200
H	-3.50203200	-1.81584800	1.87649800
N	1.89278700	-0.77062500	-0.00536100
N	-0.96038900	-1.50427600	-0.23296400

DiPip

C	0.51973000	-0.34154000	0.56303400
C	-0.51976000	-0.34154300	-0.56319500
H	0.34272300	0.49641200	1.26299800
H	0.37866800	-1.26144900	1.13835000
H	-0.37872400	-1.26145500	-1.13851800
H	-0.34277200	0.49641600	-1.26315000
C	2.30120900	1.02896900	-0.35826700
C	2.84313800	-0.88545900	1.00247100

C	3.67626100	1.01003600	-1.02811100
H	2.33040900	1.70631800	0.52228500
H	1.55571600	1.43434700	-1.04749600
C	4.24220600	-0.98468500	0.39144000
H	2.89030700	-0.27411800	1.92903800
H	2.48713800	-1.87997700	1.29071400
C	4.72401900	0.38533700	-0.09992000
H	3.96079800	2.03255100	-1.30338200
H	3.60765800	0.42683300	-1.95494400
H	4.93539100	-1.39693700	1.13428200
H	4.20661600	-1.68666200	-0.45113600
H	5.69056400	0.29633800	-0.60930200
H	4.87963400	1.04574100	0.76513000
C	-2.30116800	1.02900200	0.35817600
C	-2.84322800	-0.88547800	-1.00246400
C	-3.67615600	1.01008300	1.02815000
H	-2.33045700	1.70633800	-0.52238400
H	-1.55559700	1.43438400	1.04731900
C	-4.24223800	-0.98469100	-0.39129200
H	-2.89050800	-0.27416600	-1.92904500
H	-2.48723900	-1.87999900	-1.29071100
C	-4.72399300	0.38535800	0.10006600
H	-3.96067500	2.03260500	1.30341500
H	-3.60747400	0.42690000	1.95498900
H	-4.93549700	-1.39696500	-1.13405300
H	-4.20657100	-1.68663600	0.45130700
H	-5.69050300	0.29639400	0.60952000
H	-4.87964900	1.04572900	-0.76500200
N	1.88820900	-0.31652900	0.04923600
N	-1.88822000	-0.31651000	-0.04934300

DiPip 3-ethylallyllithium complex (syn-isomer)

C	0.26535400	2.24667500	0.13859400
C	0.61724500	1.82112600	1.41731200
C	-0.12786200	1.05008500	2.32973400
Li	-0.00414400	0.04078900	0.42996600
C	1.15521000	3.11014900	-0.71984700
C	0.80169600	4.60921600	-0.67907300
H	-0.79523500	2.26863100	-0.12363700
H	1.67448000	1.95445600	1.67212800

H	0.29935300	0.81678200	3.29927100
H	-1.21663500	1.08702300	2.29993900
H	2.19884100	2.99010400	-0.39680100
H	1.12918700	2.78253800	-1.77217900
H	1.45742900	5.20184300	-1.33108800
H	-0.23280700	4.77194900	-1.00479800
H	0.88756600	4.99455900	0.34287800
C	-0.88802200	-1.39861500	-1.71950700
C	0.26491500	-2.25464600	-1.19986900
N	1.22789500	-1.46677500	-0.40946100
N	-1.65735700	-0.76495500	-0.63352300
C	1.88808700	-2.30922400	0.61054000
C	2.23614100	-0.84482800	-1.29750400
C	-2.43070500	-1.76950600	0.12905800
C	-2.56880200	0.25145100	-1.20308800
H	-1.54240500	-2.02036300	-2.35680200
H	-0.49368300	-0.59637800	-2.35192500
H	-0.12392100	-3.05594000	-0.56677300
H	0.76072500	-2.74744800	-2.05234200
H	1.10525400	-2.74451700	1.23992400
H	2.42805100	-3.14260500	0.12210500
H	2.76513600	-1.63883600	-1.85848000
H	1.71243400	-0.21865400	-2.02575500
H	-1.73742600	-2.50002300	0.55191100
H	-3.10511200	-2.31441400	-0.55946100
H	-3.24740500	-0.22784600	-1.93423200
H	-1.95685100	0.97748600	-1.74656700
C	3.24306800	-0.00226100	-0.51809800
H	3.98364400	0.39884200	-1.21923700
H	2.71674200	0.84873400	-0.07942100
C	2.85616600	-1.49236400	1.46317500
H	2.28210300	-0.73372800	2.00880300
H	3.32041800	-2.15146100	2.20566100
C	3.91857500	-0.82156300	0.58579900
H	4.55949800	-1.59272600	0.13460100
H	4.56906600	-0.18130600	1.19168700
C	-3.24309600	-1.13145800	1.25432000
H	-3.80271900	-1.91814600	1.77322000
H	-2.55074600	-0.68957800	1.97925500
C	-3.39483100	0.95326700	-0.12617400
H	-2.72665500	1.52450200	0.52631500

H	-4.06413000	1.67317600	-0.61064300
C	-4.18783400	-0.05686100	0.70866000
H	-4.71025100	0.44888200	1.52786800
H	-4.95711600	-0.52964200	0.08135900

DiPip 3-ethylallyllithium complex (anti-isomer)

C	-0.11885400	2.45294500	-0.53045400
C	0.47135700	2.27039800	0.72323200
C	-0.04342000	1.65957800	1.87796800
Li	0.10516400	0.25809300	0.16620600
C	1.12602900	-2.26958300	-0.56818200
C	-0.06713300	-2.50122000	0.35249500
C	-1.61497600	2.57592900	-0.71699800
C	-2.16588600	3.96366400	-0.33091000
H	0.48966200	2.93301500	-1.29546000
H	1.54409200	2.47414200	0.75155700
H	0.56692800	1.62215800	2.77500300
H	-1.11753500	1.59615000	2.04391000
H	1.82530000	-3.11889100	-0.47966700
H	0.79300500	-2.25005200	-1.60951700
H	0.25447400	-2.43031600	1.39559200
H	-0.45014600	-3.52630900	0.20616200
H	-1.88831400	2.36498600	-1.76053400
H	-2.14471600	1.82891400	-0.11256300
H	-3.25560200	4.02189400	-0.45815400
H	-1.92631200	4.18681900	0.71384500
H	-1.70848100	4.74316800	-0.95047700
C	2.70703000	-1.15059900	0.88291200
C	2.58078300	-0.55954000	-1.46660000
C	3.45179500	0.13910800	1.21753100
H	3.43547800	-1.95690600	0.67052500
H	2.10980100	-1.46490600	1.74260200
C	3.31033300	0.75800800	-1.21699100
H	3.31005300	-1.34468900	-1.74426200
H	1.87957000	-0.44883800	-2.29997100
C	4.23126900	0.65694200	0.00401900
H	4.12731600	-0.05621300	2.05831800
H	2.72668000	0.88567600	1.55182800
H	3.88282800	1.01931800	-2.11439400
H	2.56378800	1.54360500	-1.06578700

H	4.68209000	1.63059800	0.22528300
H	5.05742000	-0.03343000	-0.21937100
C	-1.88247400	-1.81135900	-1.09786700
C	-2.06288600	-1.55515700	1.30825500
C	-3.03441800	-0.83838600	-1.33375300
H	-2.27429900	-2.84546400	-1.04729800
H	-1.18583500	-1.76967300	-1.93880700
C	-3.23771500	-0.59240600	1.15771600
H	-2.44405400	-2.58640500	1.43400800
H	-1.48073700	-1.29936900	2.19845400
C	-4.00284800	-0.83795000	-0.14663000
H	-3.55119100	-1.12396600	-2.25719100
H	-2.63021500	0.16628000	-1.48815200
H	-3.89792800	-0.70800500	2.02470700
H	-2.85960000	0.43403800	1.18039000
H	-4.77891400	-0.07721800	-0.28412900
H	-4.51336800	-1.81012900	-0.09420100
N	1.80688700	-0.99472000	-0.28309700
N	-1.14183900	-1.51049500	0.14805100

glyme

C	0.64529000	-0.40073900	0.00019800
H	0.68371500	-1.04742400	-0.89029900
H	0.68347600	-1.04730400	0.89078400
C	-0.64527400	0.40080600	-0.00000700
H	-0.68355100	1.04726600	-0.89066100
H	-0.68360800	1.04758000	0.89041600
C	-2.98632800	0.11506700	-0.00016300
H	-3.11895200	0.74351800	0.89381400
H	-3.74294300	-0.67228600	-0.00006300
H	-3.11877200	0.74310700	-0.89445700
C	2.98628600	-0.11514300	-0.00027400
H	3.11900900	-0.74372100	0.89360200
H	3.74299200	0.67212200	-0.00021700
H	3.11850000	-0.74309300	-0.89466900
O	-1.72205000	-0.52020200	0.00010900
O	1.72208600	0.52023800	0.00029500

glyme 3-ethylallyllithium complex (syn-isomer)

C	1.94584600	0.12822900	0.14359800
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C	1.62504500	-1.02034800	0.87247100
C	0.76812500	-1.13674600	1.97905000
C	2.91315700	0.11772800	-1.01461000
C	4.37564300	0.40514600	-0.62204300
H	1.81440200	1.09663300	0.64266300
H	1.93016900	-1.96402600	0.40584800
H	0.60755000	-2.10607100	2.43851000
H	0.59215300	-0.27390600	2.62471200
H	2.61213900	0.85016000	-1.77906100
H	2.86746500	-0.86344500	-1.50948800
H	4.46034800	1.38461100	-0.13583100
H	5.04233000	0.40272200	-1.49519200
H	4.73559000	-0.34538400	0.09057700
Li	-0.19122700	-0.15747500	0.32017800
C	-2.56814000	1.10756200	-0.41175500
H	-3.44040800	1.68397600	-0.07312300
H	-2.34875300	1.37150400	-1.45638300
C	-2.84018700	-0.37654300	-0.29044800
H	-3.68758300	-0.66028900	-0.93043000
H	-3.07457300	-0.63898400	0.75153500
C	-1.72600400	-2.47098700	-0.57192600
H	-1.87705400	-2.75206900	0.47700100
H	-0.76895800	-2.86462800	-0.91462200
H	-2.53680400	-2.86932700	-1.19513200
C	-0.99629500	2.74762500	0.33278500
H	-0.70354400	3.00568300	-0.69295600
H	-0.13046100	2.83473400	0.98938000
H	-1.78876900	3.42567400	0.67384600
O	-1.65402500	-1.05012300	-0.70240900
O	-1.43531200	1.39322900	0.40552000

glyme 3-ethylallyllithium complex (anti-isomer)

C	1.90023000	-1.16971800	-0.57767000
C	1.12641200	-2.12259300	0.08797300
C	0.62611200	-2.04625500	1.39796000
C	2.64757500	-0.09741900	0.17938900
C	3.28203700	0.95598800	-0.73450600
H	2.21857200	-1.36830300	-1.59770300
H	0.73094000	-2.92853900	-0.53614500
H	0.01641800	-2.85587300	1.78636900
H	1.12315500	-1.43394900	2.14825500

H	3.43187700	-0.53679800	0.82190000
H	1.98578700	0.41146100	0.90872700
H	3.99996600	0.48800400	-1.41737600
H	3.81681500	1.72550900	-0.16538900
H	2.52211800	1.44896700	-1.35293700
Li	-0.00418800	-0.36178300	0.10160000
C	-1.91364000	1.72006900	-0.05322300
H	-2.42886500	2.49788200	0.52759800
H	-1.88255000	2.02404600	-1.10931300
C	-2.63276500	0.39723500	0.09375800
H	-3.64969700	0.47514400	-0.31687100
H	-2.69632700	0.10824200	1.15330300
C	-2.42895200	-1.88316900	-0.57175200
H	-2.46120700	-2.24381900	0.46284000
H	-1.76824000	-2.52432800	-1.15464900
H	-3.43503100	-1.88670000	-1.01046900
C	0.20885100	2.72230000	0.35506900
H	0.31380800	3.05052700	-0.68679800
H	1.19045600	2.47539200	0.75789100
H	-0.24425500	3.52467900	0.95069400
O	-1.87368500	-0.56823000	-0.62480900
O	-0.58460700	1.54012800	0.43272000

THF

C	-1.13858000	-0.46555800	0.15335000
C	1.13334400	-0.47285600	0.16135700
C	-0.77260100	1.02037400	-0.04497800
H	-1.32772900	-0.68331800	1.21711600
H	-2.00092700	-0.79535500	-0.43026500
C	0.78144500	1.01253600	-0.05569700
H	1.99998300	-0.81548400	-0.40833900
H	1.30708400	-0.68218500	1.22960500
H	-1.16467200	1.39264000	-0.99531300
H	-1.18314700	1.64641700	0.75247900
H	1.16310900	1.36193300	-1.01893500
H	1.21064600	1.64875100	0.72367700
O	-0.00324900	-1.20504700	-0.29427800

THF 3-ethylallyllithium complex (syn-isomer)

C	-0.20637100	1.60290100	0.31986400
C	0.45966900	1.08891400	1.42967100
C	0.04726400	0.08463100	2.32527500
Li	-0.00333300	-0.63448900	0.28346900
C	0.36603800	2.69831800	-0.54367900
C	-0.09166900	4.11852100	-0.15822600
H	-1.29052800	1.46954300	0.26141000
H	1.51420100	1.37751400	1.50345600
H	0.69246700	-0.18367900	3.15542200
H	-1.01776900	-0.08128100	2.49368100
H	1.46461100	2.66069300	-0.49141800
H	0.11164000	2.53644100	-1.60435300
H	0.33449200	4.88154200	-0.82362100
H	-1.18415600	4.19863500	-0.20913400
H	0.20564100	4.34900900	0.87067300
C	2.46289500	-2.10187500	0.16256800
C	2.32038800	-0.43783600	-1.43025900
C	3.48135100	-1.05828400	0.62843100
H	2.92870600	-2.88587000	-0.45191800
H	1.89302900	-2.56186500	0.97212800
C	3.51807700	-0.03942000	-0.54116800
H	1.66823300	0.39656700	-1.69132500
H	2.64870100	-0.94786400	-2.34552700
H	3.11819800	-0.58000200	1.54105500
H	4.45931100	-1.50104400	0.83553100
H	3.40976800	0.98291600	-0.17236300
H	4.45425400	-0.09530100	-1.10348700
C	-2.30045400	-0.80935300	-1.44108300
C	-2.70691300	-1.76099500	0.62751700
C	-3.54846900	-0.08322800	-0.88693900
H	-2.57048300	-1.58659500	-2.16710200
H	-1.56496800	-0.13820000	-1.88895300
C	-3.63358900	-0.54587300	0.58975700
H	-2.23144200	-1.94088200	1.59278500
H	-3.21805600	-2.67555900	0.29354500
H	-3.44251900	1.00181100	-0.95580200
H	-4.44142900	-0.36835800	-1.45024700
H	-3.24815800	0.23003700	1.25668100
H	-4.65329200	-0.78953000	0.89964700
O	1.53368100	-1.36067800	-0.64904200
O	-1.66365000	-1.43728800	-0.30865000

THF 3-ethylallyllithium complex (anti-isomer)

C	0.32492000	-2.13749600	-0.73655100
C	-0.53673200	-2.19760700	0.36107700
C	-0.33927500	-1.70970500	1.66474600
C	1.81982200	-1.96434700	-0.58219500
C	2.55043100	-3.24264600	-0.12307700
H	-0.01927300	-2.56517400	-1.67589400
H	-1.55990000	-2.50733800	0.12901400
H	-1.12199100	-1.84136900	2.40514000
H	0.66635500	-1.59544300	2.06717600
H	2.26009400	-1.62679300	-1.53138100
H	2.04644600	-1.17336800	0.14878400
H	3.62801000	-3.07395700	0.01105100
H	2.13460900	-3.59472200	0.82635600
H	2.41958000	-4.04298000	-0.85958600
Li	-0.24051600	-0.12201300	0.13831300
C	1.60013500	1.71411600	-1.06339100
C	2.06805200	1.43705300	1.25152600
H	0.88831200	2.41629000	-1.50540700
H	1.83246000	2.33711100	1.83424500
C	-2.56313600	1.37288300	0.68469600
C	-2.78443800	0.05172400	-1.27248700
C	-4.03131800	0.95066500	0.53645000
H	-2.41987500	2.45743200	0.66174800
H	-2.10739400	0.96588900	1.59404700
C	-3.93598100	-0.30875300	-0.34056900
H	-2.24090200	-0.80408900	-1.67733400
H	-3.11908500	0.69542000	-2.09769700
H	-4.50338300	0.76467200	1.50453500
H	-4.60691100	1.72822800	0.02224100
H	-3.66685200	-1.17998400	0.26495300
H	-4.86186400	-0.52909400	-0.87890200
O	1.06899300	1.28464100	0.21683000
O	-1.85804400	0.79299200	-0.44623300
C	3.39497400	1.57565400	0.50995700
H	4.14752600	2.10992500	1.09597100
H	3.79041700	0.58712500	0.25476400
C	2.96929200	2.32840100	-0.76098100
H	3.66945700	2.20259600	-1.59090500

H	2.87355600	3.40022400	-0.55481400
H	2.00423000	0.56370400	1.90410900
H	1.67985200	0.83101900	-1.70713400

1,4-insertion transition state, TMEDA as ligand (syn-allyl, trans-butadiene)

C	3.84277700	-0.60721000	0.51022000
C	2.75629900	-1.00503000	-0.18769300
C	1.36718300	-0.75360100	0.15285700
Li	-0.57849200	0.05199500	-0.13167600
C	-2.90815900	-1.51772100	-0.37081200
C	-3.05789900	-0.67323500	0.89276800
N	-1.76262400	-0.44815800	1.56166400
N	-2.02039300	-0.87117800	-1.35564400
C	-1.88821800	0.62333300	2.56175100
C	-1.27382900	-1.67276700	2.21187200
C	-2.72868500	0.19836000	-2.07734800
C	-1.48121600	-1.85023700	-2.30753700
C	5.26627700	-0.76437700	0.05391500
C	5.98646300	0.58056800	-0.14849600
H	3.69712900	-0.12873900	1.48169000
H	2.93371300	-1.47815100	-1.15745200
H	0.69422000	-1.52251600	-0.25202000
H	1.19373900	-0.59924200	1.22174700
H	-3.90517600	-1.71182300	-0.80119600
H	-2.48018400	-2.49186900	-0.11892000
H	-3.46939400	0.30785200	0.63821300
H	-3.77730700	-1.16061100	1.57393000
H	-2.22812400	1.53753600	2.07242000
H	-2.59485300	0.35065300	3.36356500
H	-1.99779500	-2.05281700	2.95225100
H	-1.07891600	-2.45560600	1.47680400
H	-3.03022600	0.98970800	-1.38854400
H	-3.62062500	-0.19088400	-2.59656400
H	-2.27470500	-2.33536800	-2.90039700
H	-0.92425800	-2.62222200	-1.76993800
H	5.83556800	-1.35607700	0.78722300
H	5.28548100	-1.33403500	-0.88443200
H	7.03170800	0.43420100	-0.44612100
H	5.48593600	1.17394200	-0.92105700

H	5.98011400	1.16986100	0.77594800
C	1.22863000	1.28201100	-0.65878800
H	1.83081500	0.98832400	-1.51121700
H	1.83082100	1.57334700	0.19982200
C	0.01779500	1.95829600	-0.90920500
H	-0.39143400	1.92403000	-1.91796000
C	-0.69611900	2.72377100	0.07059100
H	-0.20556600	2.79292600	1.04661400
C	-1.89332000	3.36144300	-0.06488100
H	-2.42908600	3.37133200	-1.01136900
H	-2.30910400	3.95745100	0.74061800
H	-2.05863500	0.64184400	-2.81524300
H	-0.79362500	-1.34740900	-2.99234300
H	-0.91023200	0.81378100	3.01150000
H	-0.33126300	-1.46167200	2.72003000

1,4-insertion transition state, TMEDA as ligand (syn-allyl, cis-butadiene)

C	3.44869000	-0.68192400	-0.28670600
C	2.20520500	-0.27780300	-0.63178300
C	1.00148600	-1.09765400	-0.63610200
Li	-0.73524800	-0.18700300	0.32586800
C	-2.44954400	1.16140100	-1.47066600
C	-3.32920200	0.05491400	-0.89023200
N	-2.53024300	-1.11004000	-0.46994500
N	-1.42692700	1.60627300	-0.50906300
C	4.65247300	0.21592800	-0.21142800
C	5.73925700	-0.14258700	-1.24025500
H	3.62088400	-1.74040200	-0.07996300
H	2.07110500	0.78721200	-0.83115800
H	0.23434800	-0.71679800	-1.32200300
H	1.17143200	-2.15204600	-0.85229000
H	-3.08616100	2.00157300	-1.79897000
H	-1.93016500	0.79206900	-2.36047000
H	-3.86148200	0.43138400	-0.01254000
H	-4.09871100	-0.22909800	-1.62830800
H	4.33764900	1.25748900	-0.35860900
H	5.09578900	0.16762800	0.79419200
H	6.61670000	0.50715700	-1.13862000
H	6.07261700	-1.17894600	-1.11060400
H	5.35353400	-0.04491500	-2.26094000

C	0.59775000	-1.61143800	1.44777900
H	1.66408500	-1.42029800	1.55625200
H	0.35171500	-2.65245700	1.25126600
C	-0.29654100	-0.89387400	2.26821300
H	-1.23406600	-1.35630500	2.56530000
C	-0.02375900	0.43962200	2.72968900
H	-0.74693900	0.85239900	3.43583500
C	1.00708900	1.24668600	2.34115000
H	1.77666600	0.90593300	1.65601700
H	1.13131100	2.23438800	2.77467500
C	-0.36259300	2.36227000	-1.18192300
H	-0.74477700	3.28587600	-1.64847500
H	0.40184600	2.62540100	-0.44738900
H	0.09877700	1.74314700	-1.95549800
C	-2.00487800	2.42457700	0.56737500
H	-1.21090400	2.69542300	1.26480900
H	-2.47812000	3.33873900	0.17045400
H	-2.75336800	1.85594800	1.12324700
C	-3.23947700	-1.90284200	0.54055400
H	-4.18780600	-2.31398500	0.15408100
H	-2.60464900	-2.73268500	0.86013300
H	-3.45225200	-1.28258800	1.41431200
C	-2.18587800	-1.96482600	-1.61376500
H	-1.51917600	-2.76389400	-1.28242300
H	-3.08481600	-2.41370700	-2.06951000
H	-1.65961400	-1.39095800	-2.37874100

1,4-insertion transition state, TMEDA as ligand (anti-allyl, trans-butadiene)

C	-3.74672400	-0.88645500	-0.65565400
C	-2.71973000	-1.15376700	-1.49800700
C	-1.34245900	-0.70917300	-1.36054700
Li	0.44473400	-0.37821800	-0.22925800
C	2.31139300	1.65411900	-0.83517900
C	1.91764400	1.80517200	0.63223600
N	0.50106700	1.46350200	0.86385400
N	2.11953400	0.27129100	-1.31441300
C	0.23917700	1.36476500	2.30831200
C	-0.39992800	2.46723000	0.27761800
C	3.24144200	-0.58582100	-0.89666200
C	1.97335800	0.23491000	-2.77494000

C	-3.66398200	0.04347000	0.52616300
C	-4.17882600	1.46196600	0.21501200
H	-4.71890700	-1.33173600	-0.85894600
H	-2.92088600	-1.85096500	-2.31205200
H	-0.75391600	-0.78850800	-2.27765500
H	-1.26571900	0.29424800	-0.93006000
H	3.35766600	1.97698300	-0.96667200
H	1.70012400	2.31510200	-1.45531200
H	2.51895900	1.13248000	1.25151000
H	2.13474900	2.83665000	0.96156500
H	0.91194800	0.62807500	2.74869900
H	0.38238000	2.33509900	2.81281700
H	-0.19211900	3.47613200	0.67231900
H	-0.30726700	2.49219300	-0.80979500
H	3.29729100	-0.63453700	0.19234900
H	4.20010100	-0.21211000	-1.29402400
H	2.86794500	0.62172900	-3.29103700
H	1.10727700	0.82985100	-3.07590000
H	-4.24571200	-0.36627600	1.36265200
H	-2.62677400	0.10422400	0.88082700
H	-4.10154200	2.12186700	1.08861800
H	-3.61080700	1.90678700	-0.60930100
H	-5.22967000	1.43408600	-0.09268600
C	-0.63272500	-2.35575700	-0.07623600
H	-0.84569600	-3.01603700	-0.90924000
H	-1.48962200	-2.20274700	0.57689300
C	0.65487000	-2.40511000	0.49429200
H	1.46401500	-2.84654200	-0.08606300
C	0.95410100	-1.95703800	1.82242900
H	0.08668500	-1.61363300	2.39419300
C	2.16313300	-1.91430900	2.45184000
H	3.06911800	-2.27604400	1.97125100
H	2.24665700	-1.61119800	3.49021900
H	3.07853600	-1.59968900	-1.26543200
H	1.80681300	-0.79641100	-3.09613400
H	-0.79198200	1.03901400	2.46834600
H	-1.43251500	2.20780300	0.51567400

1,4-insertion transition state, TMEDA as ligand (anti-allyl, cis-butadiene)

C	3.52348900	0.56697300	-0.61799900
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C	2.19888500	0.45977200	-0.88205300
C	1.28561800	-0.59244800	-0.45537900
Li	-0.64180400	0.06487700	0.36183600
C	-2.66159200	0.01185200	-1.62693900
C	-3.15740000	-0.99923200	-0.59427200
N	-2.04180600	-1.59814700	0.15992000
N	-1.87408100	1.08730400	-1.00225500
C	4.39194100	-0.46737100	0.04763200
C	5.49838400	-0.99028500	-0.88610100
H	4.04239100	1.45968900	-0.96712400
H	1.74172200	1.30448700	-1.39741500
H	0.41746800	-0.67865700	-1.11992000
H	1.72935700	-1.57974600	-0.33783500
H	-3.52318400	0.41593900	-2.18695200
H	-2.01764900	-0.48994100	-2.35605300
H	-3.81739000	-0.50045400	0.12055200
H	-3.76418300	-1.77150200	-1.09714000
H	3.78486300	-1.30875700	0.39887200
H	4.86429400	-0.03948700	0.94355800
H	5.06426000	-1.47673600	-1.76634400
H	6.14457200	-1.71399400	-0.37529000
H	6.13023000	-0.16776900	-1.24106300
C	1.11683800	-0.38893500	1.72319300
H	2.03529900	0.18211700	1.61204300
H	1.27232500	-1.44438400	1.93160700
C	0.02177800	0.23204700	2.35562700
H	-0.69152600	-0.37371100	2.90747200
C	-0.21578300	1.64557500	2.26306800
H	-1.04840400	2.02701900	2.85715500
C	0.45573000	2.53708400	1.47445200
H	1.30762800	2.24257600	0.86962800
H	0.20544800	3.59331900	1.49515900
C	-1.09715500	1.82509300	-2.00671100
H	-1.74712800	2.33742200	-2.73599000
H	-0.47847700	2.56808700	-1.49832700
H	-0.43998300	1.13746900	-2.54491200
C	-2.72195400	2.02498800	-0.25208700
H	-2.08381400	2.77912700	0.21058900
H	-3.46033400	2.51678400	-0.90803900
H	-3.25512800	1.50719800	0.54805800
C	-2.49490400	-2.10624800	1.45944300

H	-3.25658500	-2.89757400	1.35215800
H	-1.64186000	-2.51621400	2.00505200
H	-2.91442900	-1.28861300	2.05049400
C	-1.40546200	-2.68357500	-0.59804300
H	-0.52717700	-3.03923300	-0.05506900
H	-2.09745800	-3.52863700	-0.75418000
H	-1.06900100	-2.32630000	-1.57288800

1,2-insertion transition state, TMEDA as ligand (syn-allyl, trans-butadiene)

C	3.23495900	-0.02974300	0.59474300
C	2.07578000	-0.78828100	0.51631400
C	0.87088700	-0.58740000	1.20272300
Li	-0.73688100	0.36306300	0.03500000
C	-3.39615400	-0.54540700	0.45326300
C	-2.65059000	-1.68687600	-0.23657200
N	-1.61811800	-1.19343800	-1.16498300
N	-2.49937700	0.29445000	1.26926200
C	-0.65226800	-2.25284600	-1.48501600
C	-2.21169300	-0.68726600	-2.40833400
C	-2.19113200	-0.34916000	2.55496100
C	-3.10690600	1.60791200	1.51925800
C	4.51260500	-0.42839000	-0.09442500
C	5.49295300	-1.19873300	0.80867800
H	3.34219300	0.63094300	1.45493100
H	2.07401800	-1.57029600	-0.25056000
H	0.16467800	-1.41703500	1.23580900
H	0.87851700	0.03462700	2.09831900
H	-4.21536000	-0.96257600	1.06438600
H	-3.86121400	0.09752900	-0.29898800
H	-2.15329200	-2.30858600	0.51334400
H	-3.37832900	-2.33566000	-0.75531400
H	-0.18514200	-2.61980700	-0.56984700
H	-1.12894900	-3.09919000	-2.00843400
H	-2.72999000	-1.48645100	-2.96604900
H	-2.92473000	0.11051300	-2.19794600
H	-1.73497200	-1.32693200	2.39880200
H	-3.09901100	-0.47535300	3.16902900
H	-4.04284100	1.52550600	2.09800500
H	-3.31798300	2.10314800	0.56980800
H	4.27096500	-1.04584500	-0.97160500

H	5.03355200	0.46012400	-0.48613900
H	6.42434700	-1.44022400	0.28022700
H	5.75234900	-0.60459200	1.69288900
H	5.04324100	-2.13334100	1.16116000
C	2.63652000	1.85216700	-0.71739600
H	2.86708400	1.29114700	-1.61808700
H	3.48420100	2.30593800	-0.21903300
C	1.36119600	2.32012400	-0.50284100
H	1.17052600	2.98864700	0.33601800
C	0.25414400	1.98031500	-1.33942000
H	0.49412800	1.32912000	-2.18477800
C	-1.04676000	2.38350500	-1.20312600
H	-1.33165300	3.08414500	-0.42205100
H	-1.79274000	2.15223400	-1.95460200
H	0.13304600	-1.84426900	-2.12545800
H	-1.42482400	-0.27256200	-3.04274100
H	-2.40648600	2.23017300	2.08248000
H	-1.47347600	0.26312600	3.10461000

1,2-insertion transition state, TMEDA as ligand (syn-allyl, cis-butadiene)

C	3.08687000	-0.43680500	-0.13828600
C	2.13408100	-0.40760700	-1.15194300
C	0.87609700	-1.01623000	-1.17076500
Li	-0.60284900	-0.12039700	0.13507400
C	-3.41087700	-0.55665100	-0.25931800
C	-2.93600100	0.42265700	-1.33025900
N	-1.87568300	1.31035900	-0.82280600
N	-2.31968500	-1.43733400	0.19795600
C	-1.12838500	1.92140600	-1.93085300
C	-2.42348200	2.36022300	0.04423600
C	-2.10070400	-2.54008200	-0.74984800
C	-2.61409600	-1.98481800	1.52843000
C	4.50237000	0.03074200	-0.34529700
C	5.46960400	-1.08097600	-0.79101400
H	2.94528600	-1.17831100	0.65075400
H	2.36422200	0.25361900	-1.99440200
H	0.33329800	-1.06381600	-2.11377600
H	0.71227700	-1.86668900	-0.50168400
H	-4.26165800	-1.14341400	-0.64605700
H	-3.78139500	-0.00247000	0.60760300

H	-2.52713400	-0.13127400	-2.18021600
H	-3.79663000	1.00081200	-1.71001000
H	-0.67453500	1.13807600	-2.54020100
H	-1.77546700	2.55147400	-2.56471900
H	-3.13926000	3.00289000	-0.49661000
H	-2.93304900	1.92384900	0.90572900
H	-1.84886200	-2.15254500	-1.73789100
H	-2.99483700	-3.18061300	-0.83541800
H	-3.52715000	-2.60457900	1.52665500
H	-2.74073500	-1.16899900	2.24333700
H	4.51022100	0.83390100	-1.09669300
H	4.89796000	0.47823800	0.58085200
H	6.49536900	-0.70442600	-0.89813500
H	5.48534600	-1.89677100	-0.05858400
H	5.15593700	-1.50649900	-1.75044900
C	2.37309000	1.38180800	1.21161900
H	2.84626500	0.78797300	1.98662600
H	3.03374700	2.02173800	0.63920000
C	1.03257700	1.68719200	1.29596800
H	0.64998200	2.50543200	0.68980200
C	0.08655200	1.00909200	2.14901400
H	-0.84708300	1.54393700	2.33746600
C	0.21755600	-0.21455100	2.73471600
H	1.10389000	-0.82549300	2.58679800
H	-0.53495000	-0.59077100	3.41925000
H	-0.32249000	2.53666100	-1.52539800
H	-1.60908300	2.98412100	0.41721000
H	-1.77413400	-2.59820400	1.86201500
H	-1.26073100	-3.15022500	-0.41271800

1,2-insertion transition state, TMEDA as ligand (anti-allyl, trans-butadiene)

C	-3.29237100	-0.31515200	-0.79887300
C	-2.04546200	-0.10827300	-1.38243000
C	-1.05008600	0.78593800	-0.97218400
Li	0.53391300	-0.09003300	0.29185900
C	-3.90449200	0.69356000	0.14081700
C	-4.41832600	1.96419200	-0.56045500
H	-3.97787200	-0.98723000	-1.31105900
H	-1.77671800	-0.79575100	-2.18837200
H	-0.22857700	0.98318100	-1.65937600

H	-1.31635500	1.63024700	-0.33936600
H	-4.73746500	0.23394800	0.69034200
H	-3.16351400	0.97770800	0.90170600
H	-4.82793900	2.68384600	0.16042800
H	-3.61098500	2.45368600	-1.11448200
H	-5.20882400	1.71794900	-1.27830700
C	-2.72179200	-1.92418800	0.83359500
H	-2.50423800	-2.69542900	0.10069000
H	-3.76292000	-1.82134000	1.11261100
C	-1.72392200	-1.47446500	1.66934800
H	-1.97280300	-0.78859800	2.47781900
C	-0.35688800	-1.86062700	1.52985700
H	-0.16387300	-2.60439600	0.75109600
C	0.71504700	-1.42262700	2.26138100
H	0.57842200	-0.72396800	3.08340800
H	1.69421400	-1.87563900	2.15713200
C	3.13994200	0.98989800	-0.01374200
C	2.82059200	0.24719500	-1.31058500
N	1.97814500	-0.93870500	-1.07502300
N	1.92571300	1.50392400	0.64798900
C	1.34802500	-1.39242100	-2.32197200
C	2.75586300	-2.04242000	-0.49919100
C	1.46350700	2.74758800	0.01402700
C	2.17618700	1.74955900	2.07440300
H	3.85167400	1.80612400	-0.22669900
H	3.63916200	0.31258500	0.68429600
H	2.27872900	0.91033300	-1.99098700
H	3.76390200	-0.02574100	-1.81592400
H	0.74916200	-0.58833200	-2.75183300
H	2.09537100	-1.71901900	-3.06512100
H	3.54081000	-2.39100400	-1.19239800
H	3.22772600	-1.73627100	0.43492400
H	1.25868600	2.58869900	-1.04504600
H	2.21211200	3.55175000	0.11424500
H	2.95139800	2.51916700	2.23051600
H	2.49008100	0.82264300	2.55775400
H	0.68236000	-2.23144800	-2.10517500
H	2.08958200	-2.87944300	-0.27797600
H	1.25256500	2.08800900	2.55116700
H	0.53243900	3.07076200	0.48368600

1,2-insertion transition state, TMEDA as ligand (anti-allyl, cis-butadiene)

C	-3.09379200	-0.21361700	-0.67050200
C	-2.19855200	-0.59371500	-1.67241700
C	-0.90296100	-0.13908800	-1.90272800
Li	0.33627300	-0.36893400	-0.04298600
C	2.49770400	1.44043700	0.56849600
C	2.95821900	0.60714900	-0.62422300
N	2.37189400	-0.74482100	-0.61630600
N	1.04452700	1.68746900	0.55289100
C	2.45592600	-1.35528700	-1.95021200
C	3.04983800	-1.60874900	0.35921600
C	0.69766000	2.72239500	-0.43235200
C	0.59323100	2.12582700	1.88103800
C	-2.85514400	0.98330500	0.21130400
C	-3.25377400	2.32580900	-0.43030700
H	-4.12782800	-0.53314400	-0.77445400
H	-2.51495500	-1.45029300	-2.27119200
H	-0.35641000	-0.52437500	-2.75784600
H	-0.62111200	0.86246900	-1.58641600
H	3.05991200	2.39086600	0.58701200
H	2.73584200	0.91548800	1.49775200
H	2.65719600	1.09636300	-1.55467900
H	4.06139900	0.56141100	-0.63265900
H	1.94319900	-0.72337200	-2.67707700
H	3.50199600	-1.49762200	-2.27164400
H	4.12408900	-1.71331300	0.12938400
H	2.94288300	-1.20826000	1.36832500
H	0.99504900	2.41822000	-1.43716700
H	1.18811100	3.68252300	-0.19671200
H	1.07015600	3.07436800	2.18172600
H	0.82757400	1.36073100	2.62231700
H	-1.79297000	1.02574200	0.48768300
H	-3.40282000	0.86939600	1.15792400
H	-3.04319900	3.17491900	0.23442900
H	-2.71584100	2.47916400	-1.37179200
H	-4.32448800	2.33873700	-0.66074900
C	-2.70479000	-2.10640400	0.74449300
H	-2.90765500	-1.42663900	1.56649700
H	-3.57215200	-2.57367000	0.29471800
C	-1.47055600	-2.70879000	0.62277300
H	-1.36277400	-3.53101000	-0.08013500

C	-0.28728100	-2.31599000	1.32484400
H	0.55162400	-3.00687300	1.22752300
C	-0.06890500	-1.19740800	2.08750900
H	-0.85839700	-0.47443500	2.27717100
H	0.84098800	-1.09460400	2.67066100
H	1.95587700	-2.32654000	-1.93537400
H	2.59238300	-2.59947000	0.34385600
H	-0.48921800	2.27187000	1.86808600
H	-0.38316000	2.87437800	-0.43588600

1,4-insertion transition state, TEEDA as ligand (syn-allyl, trans-butadiene)

C	-4.17344900	0.37382200	-0.65026700
C	-3.01426100	-0.25520300	-0.94149700
C	-1.67334200	0.20373100	-0.61806600
Li	0.28430000	-0.07062600	0.24726600
C	-5.54517800	-0.19826800	-0.87445300
C	-6.33675300	-0.39475700	0.43065400
H	-4.13260600	1.37430000	-0.21328300
H	-3.08673000	-1.25696600	-1.37452000
H	-0.93208200	-0.17148000	-1.33648900
H	-1.58937900	1.28723900	-0.50839900
H	-6.12615200	0.46137800	-1.53710800
H	-5.45611200	-1.16008500	-1.39636700
H	-7.34446600	-0.77954800	0.23340600
H	-5.82083700	-1.09808500	1.09295900
H	-6.43930400	0.55315200	0.97173400
C	-1.59712200	-0.46276100	1.44578000
H	-2.22399900	-1.31299600	1.20125800
H	-2.18122700	0.42499900	1.68364900
C	-0.41080300	-0.71148200	2.16911900
H	-0.03399200	-1.73248700	2.19418900
C	0.31290000	0.27564000	2.91441800
H	-0.15792300	1.26222000	2.95349200
C	1.49979800	0.13345000	3.57021100
H	2.01892800	-0.82173700	3.60603300
H	1.92467700	0.94595300	4.14996100
C	2.70671300	-0.44055800	-1.16018100
C	2.78258100	0.84708800	-0.34270400
N	1.49641100	1.57073800	-0.30079700
N	1.71418000	-1.38395600	-0.60385900

C	1.57769200	2.64686000	0.71464100
C	1.06178400	2.06434100	-1.62886900
C	2.28399400	-2.17754700	0.51408600
C	1.10920700	-2.22059000	-1.66265600
H	3.71094900	-0.88360800	-1.21489800
H	2.42193600	-0.21478800	-2.19088800
H	3.04309100	0.60929100	0.69391400
H	3.59778200	1.47573100	-0.73501500
H	2.38750400	3.35297400	0.46731800
H	1.85245300	2.15808100	1.65272700
H	0.06803100	2.49698200	-1.50377400
H	0.91583500	1.19803500	-2.27954700
H	2.68508900	-1.46712600	1.24210200
H	1.45609200	-2.67711100	1.01853200
H	0.68899500	-1.53249000	-2.40426300
H	1.87353300	-2.81774000	-2.18612500
C	-0.00215700	-3.12973900	-1.14540400
H	-0.51182900	-3.60090100	-1.99113700
H	0.38071800	-3.92912200	-0.50484200
H	-0.74196200	-2.55836600	-0.57736900
C	3.35092000	-3.21432100	0.14357800
H	3.71275400	-3.69628900	1.05724700
H	2.95163400	-3.99879400	-0.50636800
H	4.21702100	-2.77010000	-0.35642500
C	1.98101600	3.07590400	-2.32225500
H	1.53482900	3.37348200	-3.27645700
H	2.11714400	3.98185200	-1.72420100
H	2.97069600	2.66112000	-2.53702300
C	0.27068600	3.40850000	0.91045900
H	-0.56288900	2.72140200	1.08082600
H	0.35848900	4.05495200	1.78889200
H	0.02091000	4.04641000	0.05748500

1,4-insertion transition state, TEEDA as ligand (syn-allyl, cis-butadiene)

C	3.69021400	-1.32260200	-0.30227000
C	2.50744400	-0.75205200	-0.62471300
C	1.19117400	-1.36595000	-0.51951000
Li	-0.39149300	-0.16300600	0.38268300
C	5.01864300	-0.61902800	-0.34188300
C	5.98257000	-1.20493700	-1.38864000

H	3.70948900	-2.37899400	-0.02565000
H	2.53128000	0.30268800	-0.90268500
H	0.46905700	-0.92765700	-1.22114700
H	1.18371900	-2.44952900	-0.63818700
H	4.85769200	0.44731100	-0.54849000
H	5.50265700	-0.67158900	0.64468000
H	6.95241200	-0.69345900	-1.37090500
H	6.16169300	-2.27016100	-1.20100300
H	5.56199200	-1.11328800	-2.39605000
C	-1.93763300	1.26718100	-1.44049900
C	-2.95787500	0.39071800	-0.72310300
N	-2.37570200	-0.87073900	-0.22435500
N	-0.80788500	1.66660900	-0.58076300
C	-3.21676600	-1.39613800	0.87627500
C	-2.16312400	-1.85884400	-1.30957100
C	-1.20878700	2.56367100	0.53083100
C	0.25529400	2.24267400	-1.44237100
H	-2.45629100	2.14099300	-1.86583500
H	-1.51655700	0.72347100	-2.29231100
H	-3.36395300	0.92941300	0.13730500
H	-3.80954500	0.21358000	-1.39721800
H	-4.27064200	-1.46318200	0.55706500
H	-3.17723800	-0.65059500	1.67764100
H	-1.55970800	-2.67018200	-0.89625600
H	-1.53493900	-1.38502400	-2.06826300
H	-1.90319600	2.00925800	1.16953800
H	-0.31967300	2.72073900	1.14311500
H	0.61761300	1.42299900	-2.07279800
H	-0.17592200	2.99577400	-2.12355100
C	1.42749600	2.85472900	-0.68332500
H	2.25091500	3.03486100	-1.38117700
H	1.16725100	3.81413600	-0.22656200
H	1.78123000	2.19053400	0.10850900
C	-1.83338100	3.90660200	0.13759900
H	-2.02901700	4.49218000	1.04151300
H	-1.16677000	4.49562900	-0.49965700
H	-2.78566200	3.78827200	-0.38895600
C	-3.41754500	-2.43257100	-1.98065300
H	-3.11491900	-3.14393300	-2.75563000
H	-4.05706400	-2.96750600	-1.27269900
H	-4.02327200	-1.66063400	-2.46474100

C	-2.77043200	-2.74513300	1.43020600
H	-1.71789500	-2.73039000	1.71716500
H	-3.35978100	-2.97708300	2.32245800
H	-2.92198000	-3.55989500	0.71691500
C	0.81191300	-1.58904100	1.62118000
H	1.89811300	-1.58156000	1.68469900
H	0.38695100	-2.58393900	1.51781300
C	0.09331500	-0.65683600	2.39496100
H	-0.90882700	-0.90486600	2.73607700
C	0.65436300	0.59670800	2.82773400
H	0.03354400	1.17388000	3.51580700
C	1.84880800	1.13759200	2.46119700
H	2.52742900	0.62482400	1.78572400
H	2.18526000	2.08038000	2.88084400

1,4-insertion transition state, TEEDA as ligand (anti-allyl, trans-butadiene)

C	2.50319400	0.81581700	-1.16856900
C	1.90204300	1.86586800	-0.23729200
N	0.42993000	1.78288200	-0.16324400
N	2.19315700	-0.55721300	-0.71680100
C	-0.05090700	2.65695900	0.93234300
C	-0.23492500	2.06401700	-1.45774300
C	3.14272300	-1.01112300	0.33039000
C	2.09604000	-1.49266400	-1.85819600
H	3.58562900	0.98938600	-1.24431300
H	2.10793400	0.94007300	-2.17990300
H	2.27673500	1.71267900	0.78021300
H	2.24387500	2.86482800	-0.55160900
H	0.23046100	3.70613300	0.74373800
H	0.48401000	2.33822100	1.83038200
H	-1.30586200	1.91818700	-1.30999700
H	0.06298400	1.28628000	-2.16624300
H	3.12518600	-0.26260600	1.12708900
H	2.73449300	-1.92020500	0.77354400
H	1.33691900	-1.08443700	-2.53445500
H	3.03865400	-1.52665600	-2.42847100
C	1.68490800	-2.90305100	-1.44425100
H	1.47222100	-3.49822200	-2.33730500
H	2.47212900	-3.41714900	-0.88580500
H	0.78257800	-2.88253500	-0.82614100

C	4.58527900	-1.27145800	-0.11902200
H	5.18332200	-1.55988200	0.75113900
H	4.64757300	-2.08687600	-0.84599400
H	5.05690400	-0.38855900	-0.56111800
C	0.01430100	3.44461700	-2.07468000
H	-0.55888800	3.53342000	-3.00293600
H	-0.30535900	4.25297900	-1.41028700
H	1.06792400	3.60721400	-2.32180500
C	-1.55254300	2.56255500	1.18445800
H	-1.86583700	1.52268300	1.31204400
H	-1.79791700	3.10206400	2.10426100
H	-2.14662100	3.00316900	0.37847500
C	-3.87490500	-1.92370400	-0.47848600
C	-2.58027400	-1.99361600	-0.86960300
C	-1.51956200	-1.03783500	-0.60063800
Li	0.30637200	-0.29194500	0.23076600
C	-4.53341500	-0.74932500	0.19536000
C	-5.55841800	-0.04462300	-0.71209300
H	-4.52945400	-2.76250600	-0.71313500
H	-2.27015600	-2.91477600	-1.36614900
H	-0.72656600	-1.08212500	-1.35793600
H	-1.86088400	-0.01201400	-0.45772800
H	-5.04480000	-1.08403700	1.10914300
H	-3.78079000	-0.02204900	0.51980600
H	-6.05153300	0.78552600	-0.19208900
H	-5.07059000	0.35049000	-1.60980900
H	-6.33496200	-0.74496400	-1.04032800
C	-1.00691300	-1.71062700	1.42028700
H	-1.10555500	-2.74139300	1.09947300
H	-1.95438000	-1.27929300	1.73507700
C	0.16928300	-1.34010700	2.10290200
H	1.03210800	-1.99977800	2.03130700
C	0.29823300	-0.17221300	2.92419300
H	-0.62082600	0.40720200	3.05055900
C	1.41216200	0.29367800	3.55677600
H	2.35861600	-0.24014100	3.50924500
H	1.37216100	1.16683300	4.19925500

1,4-insertion transition state, TEEDA as ligand (anti-allyl, cis-butadiene)

C	3.96638000	0.42541700	-0.37116300
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C	2.64511600	0.45449400	-0.66877500
C	1.68005000	-0.63266700	-0.55175500
Li	-0.25143100	-0.07664100	0.32041600
C	4.77773900	-0.78659800	0.00247000
C	5.90153600	-1.07261200	-1.00960900
H	4.52827300	1.35552500	-0.45805100
H	2.23865700	1.42521800	-0.94697800
H	0.83945600	-0.51844900	-1.25093300
H	2.09516600	-1.63093100	-0.67810400
H	4.13290400	-1.66796000	0.08881100
H	5.22921800	-0.64362000	0.99481200
H	5.48581000	-1.27814000	-2.00202300
H	6.50654900	-1.93431000	-0.70365300
H	6.57035800	-0.20912300	-1.10385700
C	1.40672000	-0.96768200	1.58015000
H	2.38903800	-0.50982000	1.66621600
H	1.43253300	-2.05098700	1.50006200
C	0.35301700	-0.41279100	2.33500200
H	-0.45900100	-1.05634800	2.66171600
C	0.33703500	0.96165100	2.76161100
H	-0.47762200	1.23319400	3.43600000
C	1.20361300	1.94877700	2.39980600
H	2.04433200	1.75946000	1.73839100
H	1.11270500	2.94861100	2.81233200
C	-2.83798000	-0.48399900	-0.87247300
C	-2.13431900	0.66102100	-1.59216600
N	-1.27603700	1.46744700	-0.70505600
N	-1.88577000	-1.43025500	-0.25821600
C	-0.48000200	2.39278300	-1.55063800
C	-2.02823300	2.16031800	0.36893700
C	-1.40918700	-2.39793700	-1.27434300
C	-2.46855800	-2.08326000	0.93537500
H	-3.50258200	-0.98951100	-1.59105900
H	-3.48229500	-0.08400700	-0.08512900
H	-1.49071400	0.25975600	-2.38216200
H	-2.89127300	1.27992200	-2.10058500
H	-1.14038400	2.91544300	-2.26332700
H	0.18811900	1.76411100	-2.14949000
H	-1.28898700	2.66054200	0.99593300
H	-2.47385800	1.39334300	1.00983300
H	-2.26720400	-2.88633800	-1.76646700

H	-0.89337200	-1.82477600	-2.05048600
H	-1.67637600	-2.65690000	1.42125000
H	-2.73166300	-1.28199900	1.63351500
C	-3.68770500	-2.98008500	0.69112500
H	-4.04293500	-3.38202100	1.64532400
H	-4.51626500	-2.42937100	0.23439800
H	-3.44891600	-3.82921000	0.04363400
C	-0.45692500	-3.45818200	-0.73149300
H	-0.02123300	-4.01356300	-1.56732600
H	0.35794300	-3.00175800	-0.16773500
H	-0.96544500	-4.17960800	-0.08584100
C	-3.11031500	3.14763900	-0.08016100
H	-3.54622300	3.63210300	0.79934100
H	-2.70275200	3.93404300	-0.72273400
H	-3.92497800	2.65784900	-0.62304800
C	0.34290200	3.41714800	-0.77705000
H	0.89354100	2.95009800	0.04239800
H	1.06053800	3.88645200	-1.45693700
H	-0.27942000	4.21205400	-0.35548800

1,2-insertion transition state, TEEDA as ligand (syn-allyl, trans-butadiene)

C	-1.90993100	1.19631500	-1.48835700
C	-2.90226000	0.12847800	-1.03381600
N	-2.24729700	-1.04516300	-0.41751200
N	-1.05003900	1.69074700	-0.39779500
C	-3.09013700	-1.62498900	0.65292200
C	-1.87571300	-2.03630900	-1.45415100
C	-1.80663000	2.34881500	0.69095500
C	0.00953400	2.55523900	-0.96317700
H	-2.47098500	2.01134200	-1.97503000
H	-1.24892500	0.78046400	-2.25473900
H	-3.59373100	0.55869000	-0.30486800
H	-3.51395700	-0.16359300	-1.90158800
H	-3.25634100	-0.83098500	1.38684000
H	-2.50090900	-2.38828000	1.16558000
H	-1.19119200	-1.53970300	-2.14598400
H	-2.76188700	-2.32874900	-2.04206800
H	-2.48884800	1.60858000	1.11456100
H	-1.09354800	2.57287800	1.48695600
H	0.53192600	1.95741200	-1.71441400

H	-0.43177600	3.41458800	-1.49543300
C	1.02143600	3.04764600	0.06610800
H	1.84755400	3.54571800	-0.45021700
H	0.59160100	3.76871100	0.76753700
H	1.43708700	2.21019800	0.63173200
C	-2.58458000	3.61763800	0.32213500
H	-3.08928300	4.00518500	1.21291700
H	-1.92742400	4.40692400	-0.05498600
H	-3.35225600	3.42789800	-0.43458900
C	-1.19846600	-3.28209600	-0.88939900
H	-0.76342100	-3.86290000	-1.70786400
H	-0.38986300	-3.01335700	-0.20372500
H	-1.90197400	-3.93136300	-0.36021800
C	-4.43312800	-2.21872700	0.21181800
H	-4.30380700	-3.06670800	-0.46743700
H	-4.97945800	-2.57911700	1.08938900
H	-5.06371200	-1.47753500	-0.28985100
C	3.63348200	-0.77386600	-0.31221900
C	2.53337300	-0.16037400	-0.89949200
C	1.28500100	-0.73383100	-1.16465200
Li	-0.34598000	-0.19821800	0.30013600
C	4.97172900	-0.09248700	-0.20064000
C	5.93224800	-0.41108600	-1.36059200
H	3.65429200	-1.86353500	-0.31905500
H	2.62647700	0.91643700	-1.07003600
H	0.62705000	-0.21647600	-1.86157900
H	1.21668800	-1.81944500	-1.19777900
H	4.81849600	0.99514800	-0.14879700
H	5.46743200	-0.37191200	0.74276200
H	6.90627900	0.07647400	-1.22423700
H	6.10429100	-1.49139300	-1.43448700
H	5.51074100	-0.07950500	-2.31579200
C	-0.64483100	-0.33840100	2.65991500
H	-1.06780800	-1.33792800	2.71820300
H	-1.28802300	0.48590700	2.94597800
C	0.69124700	-0.15351800	2.42923200
H	1.06405100	0.87331800	2.45640300
C	1.68053400	-1.14906600	2.16572300
H	1.36218800	-2.19110900	2.16575600
C	3.00519500	-0.84423700	1.93695700
H	3.35666100	0.17387100	2.07788700

H	3.76698100	-1.61143800	2.00339500
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1,2-insertion transition state, TEEDA as ligand (syn-allyl, cis-butadiene)

C	2.99609800	-0.51694900	-0.52689400
C	2.93498600	0.71223800	0.37493900
N	1.75897600	1.56012600	0.10800500
N	1.80804800	-1.38055700	-0.36074600
C	1.65519000	2.59179500	1.16416600
C	1.75628100	2.13595100	-1.25849300
C	1.99952200	-2.34833100	0.74601800
C	1.44145800	-2.02786600	-1.64242500
H	3.92991100	-1.05866800	-0.32023000
H	3.05563500	-0.20870000	-1.57338200
H	2.86663400	0.39243400	1.42071100
H	3.87942000	1.27351100	0.28447200
H	2.56937400	3.20819200	1.19701400
H	1.60128800	2.05257200	2.11356000
H	0.81497700	2.67309300	-1.38023200
H	1.70594400	1.30828800	-1.96984200
H	2.32517200	-1.77464300	1.61913800
H	1.02239300	-2.76165400	1.00264400
H	1.27051300	-1.21857400	-2.35912900
H	2.28026700	-2.62814300	-2.03170500
C	0.17868600	-2.87789800	-1.55947000
H	-0.08374000	-3.23110200	-2.56156900
H	0.30926300	-3.75916700	-0.92454400
H	-0.65477200	-2.28579500	-1.17371100
C	2.98460100	-3.49666300	0.49310400
H	3.08332400	-4.09327400	1.40549000
H	2.63802100	-4.16366000	-0.30117600
H	3.98375500	-3.14109800	0.22287100
C	2.92710600	3.05678600	-1.61950600
H	2.78932200	3.43162400	-2.63863700
H	2.98678000	3.92356100	-0.95434300
H	3.89107900	2.53943400	-1.58725200
C	0.42905600	3.48944900	1.03830800
H	-0.48178400	2.89284000	0.94402700
H	0.33765300	4.10219300	1.94030400
H	0.49216000	4.16999100	0.18441100
C	-3.48155600	0.26716200	-0.30069100

C	-2.51228600	-0.01375300	-1.25925900
C	-1.24010300	0.54900300	-1.38248400
Li	0.23661000	0.05337300	0.13602300
C	-4.90744000	-0.19579800	-0.43400200
C	-5.83080800	0.81848000	-1.13262400
H	-3.33141900	1.16326600	0.30540300
H	-2.74179300	-0.84991200	-1.92836600
H	-0.66238000	0.34768300	-2.28306700
H	-1.07870600	1.53545500	-0.94144100
H	-4.92760500	-1.14238300	-0.99351000
H	-5.33169800	-0.42071600	0.55782100
H	-6.86595700	0.45578700	-1.17971300
H	-5.83339500	1.77405900	-0.59490200
H	-5.48749700	1.01657900	-2.15381100
C	-2.83982700	-1.22297200	1.39963500
H	-3.36477900	-0.51180000	2.02951400
H	-3.45868700	-1.97835000	0.93012900
C	-1.50119200	-1.47669900	1.61059700
H	-1.07946100	-2.38704200	1.19275800
C	-0.61875000	-0.64409300	2.39163200
H	0.30898700	-1.11725000	2.72008200
C	-0.80949400	0.65008900	2.76963800
H	-1.69690200	1.20437000	2.47807700
H	-0.10947400	1.15031200	3.43010700

1,2-insertion transition state, TEEDA as ligand (anti-allyl, trans-butadiene)

C	2.18232000	-0.43415400	-1.55014800
C	2.66571700	0.85216400	-0.88402600
N	1.59018300	1.57750600	-0.17465100
N	1.56741000	-1.38388700	-0.60445800
C	2.11744300	2.27954300	1.01806400
C	0.87631900	2.48447100	-1.10415200
C	2.50552200	-1.86190200	0.43638700
C	0.94336900	-2.49242700	-1.36079900
H	3.02757000	-0.88369200	-2.09726600
H	1.42458500	-0.19415500	-2.30212500
H	3.45463300	0.61815500	-0.16471000
H	3.13223600	1.48331700	-1.65643700
H	2.57170100	1.51616200	1.65618900
H	1.26573800	2.67008400	1.57895100

H	0.44880500	1.86465900	-1.89603100
H	1.58741200	3.17266000	-1.59117000
H	2.84749700	-0.99064800	0.99873500
H	1.92353200	-2.45426800	1.14566500
H	0.25074600	-2.03617200	-2.07227500
H	1.69917500	-3.02907200	-1.95830000
C	0.17227200	-3.47992300	-0.49143100
H	-0.36679300	-4.18163400	-1.13509500
H	0.82547300	-4.06857900	0.15935800
H	-0.56308200	-2.95855400	0.12590600
C	3.71543100	-2.67334000	-0.04225500
H	4.32288100	-2.96071600	0.82193200
H	3.41713700	-3.59185300	-0.55620600
H	4.35693400	-2.10084500	-0.71948300
C	-0.23901800	3.28618500	-0.43805300
H	-0.85560800	3.76069300	-1.20695900
H	-0.88891800	2.63964400	0.15856100
H	0.15050800	4.07762400	0.20864500
C	3.12364400	3.40531800	0.75209800
H	2.68202800	4.22345900	0.17514800
H	3.46706800	3.82114300	1.70479300
H	4.00490000	3.04728100	0.20997600
C	-3.73346800	-0.72775500	-0.36201600
C	-2.51375000	-0.91446100	-1.01069300
C	-1.50704300	0.03679000	-1.20074000
Li	0.17669700	-0.02666400	0.30282600
C	-4.30573300	0.65192400	-0.14449300
C	-4.83243100	1.31724700	-1.42881400
H	-4.44446200	-1.55110200	-0.39255500
H	-2.28111000	-1.93978200	-1.30615700
H	-0.71578600	-0.19347900	-1.91099400
H	-1.76257200	1.09034800	-1.14041300
H	-5.12354000	0.60459000	0.58747500
H	-3.53752300	1.29690700	0.30583000
H	-5.21194800	2.32827500	-1.23120100
H	-4.04078500	1.38797000	-2.18151400
H	-5.64866000	0.72898700	-1.86298900
C	0.41106100	-0.14368400	2.67976800
H	0.35419400	0.90460300	2.96195300
H	1.36010900	-0.64407400	2.83398300
C	-0.71706800	-0.84205200	2.34212600

H	-0.59766500	-1.90762200	2.13079500
C	-2.05489600	-0.35307400	2.25301600
H	-2.23181300	0.68564100	2.52880600
C	-3.11592100	-1.13674500	1.84874200
H	-2.96658500	-2.20214200	1.69856500
H	-4.13388600	-0.83391300	2.06042500

1,2-insertion transition state, TEEDA as ligand (anti-allyl, cis-butadiene)

C	2.83071500	0.63296900	-0.42894700
C	2.25324100	1.59604100	0.60446000
N	0.83174400	1.90825400	0.36852800
N	2.16207900	-0.68247700	-0.39601500
C	0.29137400	2.62559400	1.54473400
C	0.60676400	2.64351000	-0.89874300
C	2.72721800	-1.55547900	0.65941400
C	2.17821100	-1.31910400	-1.73207600
H	3.91468200	0.54896800	-0.26429800
H	2.71264100	1.04970000	-1.43209700
H	2.31994500	1.14417500	1.59947900
H	2.87487600	2.50559100	0.63541300
H	0.86763100	3.54614600	1.73898200
H	0.44871200	1.97002100	2.40509800
H	-0.47052700	2.77041300	-1.01052200
H	0.90410800	1.99053800	-1.72240200
H	2.66857700	-1.00399700	1.60238900
H	2.05583100	-2.40752600	0.77073800
H	1.69239600	-0.61709100	-2.41585500
H	3.21116400	-1.45210500	-2.09453200
C	1.43146900	-2.64845800	-1.77560900
H	1.33520500	-2.97718800	-2.81494300
H	1.95502600	-3.43822600	-1.22877100
H	0.42773700	-2.54138300	-1.35469100
C	4.15810400	-2.06509500	0.44361100
H	4.46058200	-2.66056000	1.31099900
H	4.23409300	-2.70698100	-0.43890700
H	4.88455500	-1.25411100	0.33414500
C	1.29855900	4.00441300	-1.04027900
H	1.01615600	4.45254500	-1.99821100
H	1.00100600	4.70049700	-0.25005200
H	2.38979500	3.92322700	-1.02532700

C	-1.19287800	2.96146400	1.43950600
H	-1.77661000	2.08338000	1.15108600
H	-1.55747000	3.30328200	2.41279500
H	-1.39322300	3.75730600	0.71656000
C	-3.37394500	-1.16899800	-0.78531500
C	-2.20710300	-1.10252700	-1.55317600
C	-1.25406400	-0.08809200	-1.60051400
Li	0.10888000	-0.13596400	0.13836300
C	-3.93099500	0.03539200	-0.07176200
C	-4.62871000	1.05127700	-0.99481100
H	-4.09287000	-1.93687200	-1.05976300
H	-1.97482200	-2.00510800	-2.12297100
H	-0.48588200	-0.12305400	-2.36895600
H	-1.52401700	0.90917200	-1.25880300
H	-3.12276000	0.54682700	0.47042400
H	-4.64472900	-0.28713100	0.69940200
H	-4.99652900	1.92066700	-0.43409400
H	-3.94207800	1.40600900	-1.77015200
H	-5.48381700	0.58805200	-1.49936400
C	-2.68868500	-2.51754900	1.02971200
H	-3.16423300	-1.75090600	1.63280500
H	-3.34332900	-3.28977600	0.64502500
C	-1.35220200	-2.80643600	1.22502700
H	-0.95816700	-3.73577000	0.81884200
C	-0.43125500	-1.98714400	1.94931100
H	0.49318400	-2.48794900	2.23880000
C	-0.54186700	-0.67211000	2.32372000
H	-1.44255100	-0.09587900	2.12088200
H	0.17861200	-0.23544700	3.00857100

1,2-insertion transition state, DiPyr as ligand (syn-allyl, trans-butadiene)

C	-3.98997700	0.27184600	-0.59172400
C	-2.86096300	-0.38266900	-0.94219300
C	-1.49721100	0.05690700	-0.70812700
Li	0.46682700	-0.06462300	0.11452600
C	2.67321400	-0.33848700	-1.58757000
C	2.90547800	0.92686000	-0.76536100
N	1.64097200	1.60758900	-0.46503500
N	1.85636500	-1.30519800	-0.84829200
C	1.79700800	2.67615200	0.54379400

C	1.04475500	2.28749700	-1.64349700
C	2.60520400	-2.01311300	0.22525600
C	1.28618000	-2.37001100	-1.69406100
C	-5.38250300	-0.27836200	-0.72271500
C	-6.09654300	-0.43968600	0.63106000
H	-3.90577600	1.27834400	-0.17476300
H	-2.97670600	-1.38938100	-1.35332200
H	-0.79388600	-0.35986600	-1.44082500
H	-1.38923900	1.14067600	-0.62565700
H	3.64443100	-0.77691100	-1.87574400
H	2.14666900	-0.08499100	-2.51348600
H	3.38157100	0.66889700	0.18629600
H	3.59513800	1.59775100	-1.30719900
H	2.00047600	2.23512400	1.52143600
H	2.63614200	3.34135800	0.27072100
H	1.84569000	2.71271800	-2.27066400
H	0.48069200	1.57848900	-2.25448400
H	2.62102300	-1.40912100	1.13566100
H	3.64831100	-2.17252400	-0.09253900
H	2.06472800	-2.82703400	-2.33097400
H	0.50852000	-1.96063300	-2.34570100
H	-5.99156600	0.38088800	-1.36015200
H	-5.34194500	-1.24980400	-1.23264900
H	-7.12116500	-0.80844100	0.50191400
H	-5.55361200	-1.14210000	1.27240800
H	-6.14899100	0.51835900	1.16143700
C	-1.32529400	-0.59980500	1.37502700
H	-1.88432300	-1.49806300	1.13805000
H	-1.97174100	0.24369300	1.61077800
C	-0.10801400	-0.74547400	2.06891800
H	0.35170600	-1.73135300	2.09730000
C	0.54593700	0.30520700	2.79361500
H	0.00671500	1.25718600	2.81740300
C	1.73986500	0.25375700	3.44748100
H	2.32272900	-0.66356900	3.49627500
H	2.11558800	1.10406400	4.00643200
C	0.15269900	3.41057200	-1.06260700
H	0.40497000	4.36812700	-1.52652400
H	-0.90657100	3.22545000	-1.25484600
C	0.46932700	3.42350600	0.45318000
H	-0.29749000	2.87616100	1.01017100

H	0.52766900	4.43290300	0.86791400
C	1.87817000	-3.36738200	0.41054400
H	2.57776300	-4.19244800	0.24833600
H	1.47023600	-3.48011200	1.41716300
C	0.76824500	-3.37189100	-0.66598200
H	0.59169300	-4.36222800	-1.09305300
H	-0.17476100	-3.00704000	-0.24761300

1,2-insertion transition state, DiPyr as ligand (syn-allyl, cis-butadiene)

C	3.63260700	-1.17782700	-0.23528600
C	2.45774100	-0.62155900	-0.60770000
C	1.14954300	-1.26074200	-0.57045900
Li	-0.53153100	-0.15700200	0.31769200
C	-2.00313400	1.25073700	-1.57503800
C	-3.03504400	0.31667800	-0.94789800
C	4.95240000	-0.45783500	-0.20937100
C	5.96959500	-1.02405500	-1.21579400
H	3.65395200	-2.23654000	0.03222900
H	2.47856900	0.43710800	-0.87319700
H	0.44145700	-0.80495700	-1.27540900
H	1.17269100	-2.33694500	-0.73922100
H	-2.52311000	2.11624500	-2.02148200
H	-1.48210400	0.73019100	-2.38487900
H	-3.51435800	0.82294300	-0.10424900
H	-3.82955200	0.09013600	-1.67977800
H	4.78780600	0.60811500	-0.41506900
H	5.39158600	-0.51279700	0.79773400
H	6.93114400	-0.50097400	-1.15052800
H	6.15346200	-2.08841800	-1.02785300
H	5.59381900	-0.92962800	-2.24047400
C	0.70679600	-1.59571200	1.54255900
H	1.78572700	-1.49890000	1.64789300
H	0.36767200	-2.61870400	1.40389300
C	-0.11539700	-0.75012700	2.31309000
H	-1.09774900	-1.09648300	2.62553700
C	0.30543200	0.56241400	2.72623300
H	-0.36413400	1.08070800	3.41560500
C	1.42795000	1.22393800	2.32232600
H	2.15008100	0.77252900	1.64913700
H	1.67202200	2.20165300	2.72566100

C	0.17028200	2.37113000	-1.17078900
C	-1.59139700	2.58754000	0.45057800
C	-0.01125400	3.85353800	-0.83506800
H	0.23760200	2.15943800	-2.24097900
H	1.07741100	1.99580800	-0.68930400
C	-0.62060700	3.76987900	0.56976700
H	-1.72854100	2.06706600	1.40211600
H	-2.57438600	2.93970700	0.10691200
H	0.93116500	4.40750700	-0.86646000
H	-0.70954400	4.33042600	-1.53429800
H	0.15850000	3.53303700	1.29972900
H	-1.12889600	4.68544900	0.88535000
C	-3.25859600	-1.60540100	0.55287600
C	-2.20180100	-1.93803800	-1.48980300
C	-2.64662900	-3.00944900	0.66246300
H	-4.30089600	-1.66413000	0.19202200
H	-3.25438300	-1.05041600	1.49504600
C	-1.94013200	-3.23249700	-0.70423200
H	-1.37551500	-1.66305500	-2.14946000
H	-3.11277100	-2.03423100	-2.10737300
H	-1.92332300	-3.04862700	1.47972100
H	-3.41450000	-3.76035400	0.86498100
H	-0.86836500	-3.38304700	-0.56377200
H	-2.32885600	-4.10183100	-1.24061000
N	-1.00510200	1.66448100	-0.57592700
N	-2.41621600	-0.91486700	-0.44449700

1,2-insertion transition state, DiPyr as ligand (anti-allyl, trans-butadiene)

C	-3.52204600	-1.94241200	-1.05950700
C	-2.19579000	-2.05747300	-1.31273100
C	-1.14525300	-1.10517300	-1.00545200
Li	0.42550000	-0.14128200	0.04523800
C	2.56092800	1.06277400	-1.32531000
C	1.92514400	2.14544400	-0.45663700
N	0.47469900	1.95553800	-0.34645400
N	2.37362400	-0.26611000	-0.73504600
C	-0.13757500	2.82785700	0.67684100
C	-0.25744700	2.27868300	-1.59779400
C	3.27728000	-0.52932000	0.41793700
C	2.61759400	-1.37281000	-1.67861000

C	-4.21637000	-0.73546100	-0.48894700
C	-4.96800100	-1.03261200	0.82014400
H	-4.16615600	-2.78873300	-1.29611400
H	-1.86085200	-3.01415000	-1.71678700
H	-0.25521000	-1.23668100	-1.63143100
H	-1.47159400	-0.06459700	-0.99106300
H	3.63239200	1.28509800	-1.46956300
H	2.09558000	1.06469100	-2.31630000
H	2.34570000	2.10667200	0.55359200
H	2.16167800	3.13971900	-0.87487000
H	0.16911700	2.50303200	1.67243300
H	0.18476900	3.87473200	0.53042600
H	0.21715500	3.14217300	-2.09259900
H	-0.22681300	1.43546600	-2.29258300
H	2.85170900	-0.11296700	1.33373400
H	4.24979600	-0.04069000	0.24483300
H	3.58116300	-1.23891900	-2.20226600
H	1.82341300	-1.41208400	-2.43012700
H	-3.49544900	0.07041400	-0.31226800
H	-4.93950400	-0.34288900	-1.22114700
H	-5.50108500	-0.14644500	1.18482500
H	-5.70417600	-1.83137400	0.67453800
H	-4.27498200	-1.36421200	1.60064900
C	-0.85616300	-1.66765700	1.12160100
H	-0.82607600	-2.70780200	0.81895600
H	-1.86697200	-1.30283300	1.28403000
C	0.18394500	-1.17619600	1.93007100
H	1.10268000	-1.75524100	1.99748100
C	0.09551000	0.01520100	2.72425900
H	-0.87523500	0.51939200	2.69440700
C	1.06215500	0.57778400	3.50134100
H	2.04272000	0.11986300	3.61123800
H	0.86376700	1.46064700	4.09952900
C	-1.69757400	2.62883200	-1.15191800
H	-1.99488100	3.59531500	-1.56805100
H	-2.42174300	1.88932600	-1.50115200
C	-1.63060000	2.68323200	0.39415300
H	-1.99784500	1.74742500	0.82769700
H	-2.21917600	3.50070500	0.81780100
C	3.44267300	-2.06759900	0.46922800
H	4.50156600	-2.33246000	0.39841000

H	3.06368400	-2.49068700	1.40181600
C	2.66386300	-2.59082900	-0.76000900
H	3.13805300	-3.45620700	-1.22964400
H	1.64441100	-2.87144300	-0.47760600

1,2-insertion transition state, DiPyr as ligand (anti-allyl, cis-butadiene)

C	-3.70416000	-0.63687900	-0.46264000
C	-2.37915700	-0.60690900	-0.74337700
C	-1.46593000	0.52366700	-0.62548100
Li	0.46803800	0.06862800	0.27713800
C	-4.57484800	0.54059600	-0.11298800
C	-5.69050700	0.77083900	-1.14813100
H	-4.22143500	-1.59261500	-0.54745300
H	-1.92338800	-1.56144400	-1.00533300
H	-0.61212100	0.43793300	-1.31125600
H	-1.92167300	1.50262900	-0.76463100
H	-3.97091700	1.44990500	-0.02096700
H	-5.03843600	0.38420500	0.87167900
H	-5.26511100	0.98780600	-2.13397500
H	-6.33799500	1.60740700	-0.85987600
H	-6.31938700	-0.12145500	-1.24866600
C	-1.23395200	0.89489800	1.50759400
H	-2.19869100	0.39990800	1.58606200
H	-1.29954400	1.97439900	1.40721600
C	-0.17075500	0.38669400	2.28056000
H	0.61560600	1.05968900	2.61168200
C	-0.10650200	-0.98699500	2.70735100
H	0.70096700	-1.22631900	3.40241800
C	-0.92694400	-2.00528700	2.32542000
H	-1.75668800	-1.84858700	1.64255700
H	-0.80916700	-3.00074400	2.74151300
C	2.49414600	-0.50259100	-1.58466300
C	3.04732800	0.64876900	-0.75288900
N	1.97902400	1.52727400	-0.26638900
N	1.60826900	-1.36476600	-0.79506200
C	2.44233300	2.42526400	0.81089700
C	1.46302600	2.45604700	-1.29483400
C	2.33710300	-2.17256600	0.22782400
C	0.88392300	-2.33636400	-1.64383200
H	3.33340100	-1.08352500	-2.00685100

H	1.91964900	-0.10872900	-2.42983800
H	3.57744200	0.24663600	0.11667800
H	3.78535500	1.21610000	-1.34682800
H	2.58782600	1.85899600	1.73456000
H	3.40913500	2.87968300	0.53041400
H	2.30812400	2.92123800	-1.83354000
H	0.84367000	1.93318400	-2.02716100
H	2.33781800	-1.64471100	1.18550900
H	3.38403200	-2.31424200	-0.08162900
H	1.56744700	-2.78062500	-2.38918600
H	0.07495200	-1.83326300	-2.18145600
C	0.68352600	3.50850500	-0.49246000
H	0.73091600	4.48712900	-0.97671000
H	-0.36822300	3.22584900	-0.41961100
C	1.35137600	3.50201200	0.91105600
H	0.62392300	3.24194100	1.68283400
H	1.77941700	4.47232900	1.17512000
C	1.59874900	-3.52838400	0.31470200
H	2.26492200	-4.33846200	0.00201200
H	1.26395600	-3.73720100	1.33211800
C	0.40783500	-3.39377800	-0.65460700
H	0.14597700	-4.33527800	-1.14460500
H	-0.46646600	-3.02843900	-0.11107900

1,4-insertion transition state, DiPip as ligand (syn-allyl, trans-butadiene)

C	3.55230900	-1.86853700	-0.65074000
C	2.64776000	-0.92001700	-0.97802600
C	1.23003800	-0.92609700	-0.65142900
Li	-0.45044600	0.12341600	0.17732000
C	-2.18161700	2.00422800	-1.02211900
C	-2.97100800	0.91224900	-0.30656300
C	5.03335200	-1.76370400	-0.88427300
C	5.85097900	-1.77752500	0.41944400
H	3.20206100	-2.78943600	-0.17894600
H	3.03193000	-0.01300100	-1.45172000
H	0.64620400	-0.34830200	-1.38302600
H	0.80216700	-1.92271500	-0.52487800
H	-2.73119500	2.95614500	-0.94926000
H	-2.11387000	1.77200100	-2.08748500
H	-3.00589900	1.12261700	0.76783300

H	-4.01403100	0.92230800	-0.66932500
H	5.37565700	-2.59613400	-1.51791200
H	5.24851900	-0.84235600	-1.44137800
H	6.92782500	-1.73551700	0.21688100
H	5.58368700	-0.92416300	1.05183100
H	5.65287400	-2.68915800	0.99505900
C	1.32244700	-0.36269000	1.42018400
H	1.84717900	-1.30676000	1.54551100
H	2.00744100	0.46057300	1.23693500
C	0.18157200	-0.11880500	2.21681000
H	-0.10306100	0.90849900	2.44132100
C	-0.53632300	-1.15651000	2.90178300
H	-0.16044900	-2.16907800	2.73081000
C	-1.60154600	-1.02612800	3.73531800
H	-2.02221900	-0.05048900	3.97200200
H	-2.03944500	-1.88513000	4.23210700
C	0.10196500	2.60700500	-1.56637200
C	-0.80464600	3.11513400	0.63288600
C	1.52720100	2.81068100	-1.06003500
H	-0.27447000	3.55224800	-1.99997100
H	0.08506600	1.85344000	-2.36068200
C	0.59465200	3.37391900	1.19142100
H	-1.23782600	4.07229000	0.28707000
H	-1.46068200	2.72684900	1.41791200
C	1.55646600	3.82337100	0.08801600
H	2.15506800	3.14249500	-1.89446300
H	1.92480700	1.85048000	-0.71641100
H	0.51716600	4.13262500	1.97820600
H	0.98011600	2.46623400	1.66322300
H	2.57187400	3.92686100	0.48504300
H	1.25583100	4.81201900	-0.28662900
C	-3.01953600	-1.37510800	0.45561100
C	-2.51694900	-0.90076300	-1.86931000
C	-2.41693200	-2.77114100	0.34081000
H	-4.10333100	-1.41789000	0.23809200
H	-2.88814000	-1.00114600	1.47382400
C	-1.93701100	-2.30111300	-2.07206800
H	-3.58976200	-0.89829700	-2.14042600
H	-2.01181700	-0.20200400	-2.54079300
C	-2.54069700	-3.30724100	-1.08797300
H	-2.91821800	-3.43037100	1.05759400

H	-1.36283800	-2.72569900	0.63705700
H	-2.12403000	-2.60608700	-3.10816300
H	-0.85079300	-2.26120300	-1.94254500
H	-2.04479600	-4.27939800	-1.18408400
H	-3.60191200	-3.46465700	-1.32763300
N	-0.80852500	2.14979600	-0.49219400
N	-2.36864800	-0.42353600	-0.47563200

1,4-insertion transition state, DiPip as ligand (syn-allyl, cis-butadiene)

C	3.12224200	-2.23149900	-0.26335100
C	2.17503300	-1.33693900	-0.62622000
C	0.73411500	-1.53996300	-0.58450000
Li	-0.49346400	0.08277300	0.26993200
C	-1.42367400	1.63494500	-1.81306100
C	-2.72054500	1.17173400	-1.15925800
C	4.59875200	-1.94834400	-0.23364400
C	5.39617900	-2.78474900	-1.24984200
H	2.81785100	-3.24742200	-0.00242800
H	2.52317400	-0.33693300	-0.88801000
H	0.19372800	-0.93024300	-1.32180100
H	0.43076900	-2.58005200	-0.69993800
H	-1.62806100	2.53055100	-2.42564300
H	-1.05651700	0.86342800	-2.49762400
H	-3.04398900	1.90800900	-0.41973500
H	-3.51547700	1.13111700	-1.92275200
H	4.76646400	-0.88047000	-0.42661700
H	5.00048000	-2.14595100	0.77128900
H	6.47131100	-2.57996700	-1.18144300
H	5.24714600	-3.85680100	-1.07528000
H	5.06746600	-2.56780400	-2.27210700
C	0.92742900	2.08049200	-1.55454800
C	-0.66822200	3.14439600	-0.06919800
C	2.07942300	2.42135500	-0.61293800
H	0.81677500	2.88049300	-2.31057700
H	1.13304500	1.15006600	-2.09275600
C	0.44191000	3.52803500	0.90575600
H	-0.84277500	3.97232000	-0.78269500
H	-1.59869200	2.98978100	0.48230900
C	1.78075500	3.69380200	0.18331200
H	2.99594300	2.52814000	-1.20429200

H	2.23328500	1.59597100	0.08902000
H	0.15018900	4.45324300	1.41627400
H	0.53959800	2.74613700	1.66396500
H	2.58118300	3.88746300	0.90508000
H	1.73722100	4.55954500	-0.49334200
C	-3.62313100	-0.24476900	0.56969100
C	-2.73694300	-1.22358000	-1.47006800
C	-3.61382200	-1.60351100	1.26700700
H	-4.62067600	-0.07291900	0.12276800
H	-3.44771900	0.55524900	1.29650600
C	-2.69761900	-2.61030300	-0.83290800
H	-3.69892100	-1.09514900	-2.00161600
H	-1.94095600	-1.13142900	-2.21404300
C	-3.76573900	-2.74345200	0.25582200
H	-4.42502400	-1.62241500	2.00354400
H	-2.67720500	-1.72314600	1.81949500
H	-2.84314400	-3.35860500	-1.62002800
H	-1.70703800	-2.78247000	-0.40521400
H	-3.68649500	-3.71421700	0.75687800
H	-4.76452100	-2.69922300	-0.20102800
N	-0.35647000	1.91072700	-0.83187500
N	-2.58408400	-0.13162400	-0.47975300
C	0.19550700	-1.62409300	1.54557100
H	1.21047300	-2.00227500	1.64466600
H	-0.55416400	-2.39764700	1.40587400
C	-0.17064900	-0.50106600	2.30850600
H	-1.20788100	-0.37557900	2.61236300
C	0.79424600	0.43849600	2.82326800
H	0.39898500	1.16923300	3.53163400
C	2.11839200	0.51308500	2.52333400
H	2.58966800	-0.17157700	1.82471200
H	2.75692900	1.24507700	3.00780100

1,4-insertion transition state, DiPip as ligand (anti-allyl, trans-butadiene)

C	-2.86392600	-2.99636000	-0.35245000
C	-1.66857400	-2.49476200	-0.74340700
C	-1.14048200	-1.16012100	-0.50563600
Li	0.40678700	0.13464700	0.18788100
C	2.64352500	1.20158200	-1.16941900
C	1.87681800	2.29099400	-0.42547700

C	-3.99141800	-2.22371400	0.27833300
C	-5.24045600	-2.16789000	-0.61977700
H	-3.07031400	-4.04669600	-0.55701800
H	-0.98013600	-3.19740000	-1.21585300
H	-0.42501100	-0.87101300	-1.28870000
H	-1.89363500	-0.38209900	-0.37413100
H	3.71843200	1.44150100	-1.15649700
H	2.34569500	1.19356800	-2.22044600
H	2.14668700	2.27601300	0.63607800
H	2.17664700	3.27832200	-0.81904200
H	-4.26944500	-2.68546900	1.23676800
H	-3.67170500	-1.20296900	0.51569300
H	-6.06282500	-1.63367900	-0.12939700
H	-5.01442800	-1.66147000	-1.56437100
H	-5.59216900	-3.17738200	-0.86210100
C	-0.49696900	-1.37851300	1.54260500
H	-1.54337500	-1.58160000	1.75043400
H	0.06214600	-2.28650700	1.33615100
C	0.13752000	-0.34586600	2.26696400
H	1.21761600	-0.37506600	2.40537200
C	-0.58301700	0.66812600	2.98392900
H	-1.67147700	0.61254400	2.89496800
C	-0.07677700	1.66330700	3.75834100
H	0.99490800	1.77364800	3.91366500
H	-0.72495000	2.35293500	4.28814900
C	2.48692400	-1.16405600	-1.67956300
C	3.39091800	-0.43201700	0.45627200
C	2.27683000	-2.57739300	-1.14283400
H	3.47200300	-1.10130100	-2.17839500
H	1.72544700	-0.92510800	-2.42935700
C	3.24558100	-1.83641800	1.04223900
H	4.40940200	-0.31802400	0.04030400
H	3.27511000	0.32128800	1.24157000
C	3.30425700	-2.90293500	-0.05504200
H	2.34708000	-3.28600800	-1.97555900
H	1.26495500	-2.65782800	-0.73255900
H	4.04242900	-1.98710100	1.77912100
H	2.29736000	-1.91817500	1.57997300
H	3.11725500	-3.89599600	0.36711300
H	4.31066500	-2.92600300	-0.49635500
C	-0.24856700	3.03289100	0.44118900

C	-0.07277500	2.37258200	-1.88525200
C	-1.76416400	2.86555100	0.41523000
H	0.01541500	4.07677300	0.18744300
H	0.12830100	2.81775900	1.44391000
C	-1.59076500	2.22988000	-2.00298400
H	0.23100300	3.39214500	-2.18972000
H	0.40793500	1.67264900	-2.57310100
C	-2.32020600	3.11639800	-0.98925400
H	-2.20646900	3.55171000	1.14544800
H	-2.01307200	1.85034400	0.74481700
H	-1.88351300	2.48562200	-3.02786400
H	-1.86480000	1.18190900	-1.84560700
H	-3.39843700	2.92508900	-1.02182100
H	-2.17506600	4.17331000	-1.25419200
N	2.40031300	-0.14544900	-0.60857600
N	0.41516000	2.11233800	-0.51179200

1,4-insertion transition state, DiPip as ligand (anti-allyl, cis-butadiene)

C	-3.71061500	-1.20474500	-0.46823300
C	-2.39386300	-1.04658100	-0.74538100
C	-1.59817800	0.16898200	-0.62841900
Li	0.41356700	0.07660600	0.27266800
C	-4.69240200	-0.11774300	-0.11961000
C	-5.81845700	0.00965300	-1.16126300
H	-4.13247600	-2.20617400	-0.55381700
H	-1.84843100	-1.95208400	-1.00753600
H	-0.74846500	0.17731600	-1.32439100
H	-2.15788300	1.09335100	-0.75912300
H	-4.17936900	0.84507300	-0.01965900
H	-5.14506500	-0.32256500	0.86128600
H	-5.40945100	0.27191600	-2.14304200
H	-6.54570600	0.77822300	-0.87366300
H	-6.35738800	-0.93869200	-1.27057100
C	-1.39045100	0.53007600	1.52672000
H	-2.31392400	-0.03888700	1.58791100
H	-1.53682300	1.60269200	1.43882300
C	-0.29516100	0.08723400	2.29121500
H	0.44037100	0.80868900	2.64074200
C	-0.16424700	-1.27488800	2.74455000
H	0.64184500	-1.45115600	3.45951900

C	-0.91940300	-2.34516800	2.37931800
H	-1.73638800	-2.25847100	1.66912900
H	-0.74720300	-3.32237300	2.81930100
C	2.67215700	1.20448100	-1.06175500
C	2.23784100	-0.05981200	-1.79448800
H	3.15225100	1.89098400	-1.77924900
H	3.43381500	0.95641300	-0.31870300
H	1.42076700	0.17301600	-2.48494900
H	3.07757000	-0.42672000	-2.41035000
C	2.09825500	2.70585700	0.73349600
C	0.81160400	2.72261300	-1.32923100
C	1.02062200	3.51496100	1.45223100
H	2.86344800	3.39715600	0.33241900
H	2.60062700	2.03421800	1.43749300
C	-0.30294700	3.53109900	-0.66958500
H	1.52007700	3.41584700	-1.82098800
H	0.39453600	2.07842000	-2.10808100
C	0.24548400	4.39562400	0.46824700
H	1.50063700	4.12208000	2.22801800
H	0.33064100	2.83416400	1.95976900
H	-0.78443300	4.14835600	-1.43629400
H	-1.06315000	2.84838700	-0.28268900
H	-0.56830800	4.91993200	0.98064400
H	0.91413600	5.16518900	0.05729300
C	1.10224300	-2.17940800	-1.67097300
C	2.90864100	-1.69188100	-0.12788100
C	0.62325300	-3.33495600	-0.79660300
H	1.80720100	-2.55805900	-2.43480100
H	0.25989100	-1.72498400	-2.20150200
C	2.49106600	-2.84496000	0.78125900
H	3.67205400	-2.04078000	-0.84932200
H	3.36706000	-0.90262800	0.47292100
C	1.78511000	-3.94783600	-0.01098700
H	0.13822100	-4.08136400	-1.43585400
H	-0.12649600	-2.96901400	-0.08825800
H	3.38508300	-3.23018000	1.28532900
H	1.81177900	-2.46758800	1.55066100
H	1.41803800	-4.72661300	0.66567000
H	2.49456000	-4.42594700	-0.70190800
N	1.55570100	1.87562800	-0.36676100
N	1.76606200	-1.11599600	-0.87837400

1,2-insertion transition state, DiPip as ligand (syn-allyl, trans-butadiene)

C	3.15335800	-1.73244800	-0.27085100
C	2.27394000	-0.88278300	-0.93018400
C	0.90720800	-1.09023400	-1.14869800
Li	-0.47475000	0.02250200	0.21756900
C	-2.87639100	0.93976800	-0.94535100
C	-1.71382100	1.66407100	-1.61827300
N	-0.62967000	2.00922900	-0.68000800
N	-2.51843900	-0.40100300	-0.44014800
C	0.57590300	2.39950500	-1.44440000
C	-1.04430500	3.12513200	0.19974800
C	-2.55776600	-1.38727100	-1.54618800
C	-3.47785500	-0.78931500	0.61833900
C	4.63317800	-1.46479900	-0.19708800
C	5.44970900	-2.17250700	-1.29349900
H	2.85202600	-2.77453100	-0.16702900
H	2.67750000	0.09457700	-1.21122600
H	0.40930000	-0.48993500	-1.90953500
H	0.53303100	-2.10747300	-1.06098300
H	-3.71622000	0.87259700	-1.65778200
H	-3.23633200	1.53057500	-0.09946400
H	-1.28786200	1.03131400	-2.40247100
H	-2.09983900	2.57051600	-2.11794200
H	0.85449700	1.56193600	-2.08748200
H	0.33731600	3.25775000	-2.10119900
H	-1.35898600	3.98237700	-0.42610000
H	-1.91411100	2.80941500	0.78010800
H	-1.81746700	-1.09941500	-2.29631400
H	-3.55219200	-1.34669600	-2.02978200
H	-4.50923800	-0.74393600	0.22013800
H	-3.40036200	-0.05059700	1.42079000
H	4.80654100	-0.38092400	-0.26238300
H	5.03176600	-1.77477300	0.78218400
H	6.52489600	-1.98006000	-1.18434700
H	5.29610500	-3.25724900	-1.25048800
H	5.13770900	-1.83570200	-2.28808900
C	2.55068500	-1.40073400	1.97934700
H	3.19261700	-0.52553500	2.00895700
H	3.04923100	-2.34952600	2.13596800

C	1.19972600	-1.26860900	2.21530500
H	0.58488500	-2.15953800	2.33749800
C	0.56316700	0.00487600	2.32596000
H	1.23320200	0.85792900	2.19528100
C	-0.75514700	0.27648800	2.57491100
H	-1.45849700	-0.52073800	2.79514400
H	-1.10506700	1.29221000	2.72140000
C	0.06405500	3.57548000	1.15173500
H	-0.30256200	4.43226400	1.72864500
H	0.27329200	2.77565400	1.86724300
C	1.73518900	2.77116900	-0.52365800
H	2.00854200	1.89409500	0.07299100
H	2.60671300	3.02805800	-1.13602600
C	1.34606100	3.93192600	0.39487400
H	1.18001000	4.83582100	-0.20797900
H	2.15481600	4.16085900	1.09741300
C	-2.28825600	-2.81502800	-1.07212200
H	-2.35638100	-3.48685800	-1.93494700
H	-1.26503300	-2.88140200	-0.69182800
C	-3.21138400	-2.19253900	1.15729000
H	-2.22101400	-2.21732900	1.62650600
H	-3.94640000	-2.41666800	1.93863100
C	-3.26544600	-3.22717800	0.03068200
H	-3.02005700	-4.22529800	0.40932700
H	-4.28621000	-3.27868300	-0.37371900

1,2-insertion transition state, DiPip as ligand (syn-allyl, cis-butadiene)

C	3.43856000	-0.35227600	-0.26329600
C	2.50892900	0.10638400	-1.18729500
C	1.18380600	-0.31415500	-1.34414500
Li	-0.35786500	0.01644900	0.12641400
C	-3.10878900	-0.60109100	-0.11595600
C	-2.87217500	0.57542100	-1.05493600
N	-1.84935700	1.50737300	-0.54441700
N	-1.96729000	-1.53547400	-0.06191700
C	-1.29407400	2.29439700	-1.67004800
C	-2.45695000	2.42134000	0.45014600
C	-1.92534800	-2.34683200	-1.30452300
C	-2.14156200	-2.41971300	1.11298300
C	4.89876800	0.00475000	-0.32674900

C	5.75745600	-1.01678500	-1.09454300
H	3.19841900	-1.27643100	0.26632600
H	2.82437300	0.96221600	-1.79321100
H	0.64938900	-0.03000100	-2.24955100
H	0.93951000	-1.30788800	-0.96301700
H	-4.02761200	-1.13238900	-0.42089600
H	-3.28429700	-0.23056700	0.89889100
H	-2.53917400	0.20931800	-2.02939100
H	-3.82660100	1.10106100	-1.22878900
H	-0.86159000	1.59076900	-2.38497300
H	-2.11250900	2.83605800	-2.18123900
H	-3.31933600	2.93500600	-0.01586000
H	-2.84876500	1.82529600	1.27983300
H	-1.72526600	-1.68234300	-2.14851700
H	-2.92279900	-2.79722200	-1.46877400
H	-3.12914300	-2.91626100	1.05842500
H	-2.14081900	-1.78694000	2.00468400
H	5.00802800	0.99157800	-0.79942600
H	5.31397800	0.10740500	0.68875700
H	6.81904900	-0.73688200	-1.08915700
H	5.66987700	-2.01253000	-0.64375500
H	5.42640800	-1.09670700	-2.13568400
C	2.85816500	1.02658200	1.60033400
H	3.25531400	0.19270900	2.16990900
H	3.58790100	1.74106200	1.23964600
C	1.54276900	1.40204200	1.73057300
H	1.25200700	2.37565100	1.34932000
C	0.51175400	0.61238200	2.35687600
H	-0.40057700	1.15183400	2.62383900
C	0.54227300	-0.71372200	2.66693900
H	1.40562100	-1.33195100	2.43791200
H	-0.26429800	-1.17738400	3.22372900
C	-1.47535500	3.46682300	0.97846800
H	-2.01846500	4.14161600	1.65009000
H	-0.70612100	2.97610700	1.57813900
C	-0.23336400	3.28267700	-1.19873400
H	0.60091400	2.71524700	-0.77247700
H	0.15231900	3.82966500	-2.06646000
C	-0.81646600	4.24929300	-0.16266100
H	-1.56633900	4.89149800	-0.64609500
H	-0.03772500	4.91103200	0.23177800

C	-0.87563900	-3.45872800	-1.27756500
H	-0.97400000	-4.03967900	-2.20169700
H	0.12592500	-3.01971100	-1.28806900
C	-1.05000400	-3.48050100	1.21048800
H	-0.08193800	-2.98351000	1.33442900
H	-1.22329400	-4.08338400	2.10915500
C	-1.03229900	-4.35327800	-0.04628000
H	-0.21925500	-5.08573500	0.00041700
H	-1.97172700	-4.92031200	-0.11359400

1,2-insertion transition state, DiPip as ligand (anti-allyl, trans-butadiene)

C	-2.24592300	-2.92255400	-0.47785500
C	-1.02023300	-2.56304900	-1.03034300
C	-0.56182900	-1.27581000	-1.33688700
Li	0.35548400	0.05116700	0.21204100
C	1.20428400	2.69749000	-0.31586300
C	2.05274800	1.81533800	-1.22494000
N	2.36237600	0.49966500	-0.63741100
N	-0.15057800	2.16663400	-0.07111100
C	2.85141200	-0.40389700	-1.70167500
C	3.40081800	0.61913000	0.40981000
C	-1.01319800	2.37305700	-1.25951000
C	-0.72957200	2.87709100	1.09106000
C	-3.40033000	-1.95758800	-0.40409600
C	-4.06761400	-1.65589200	-1.75832700
H	-2.48056000	-3.98304200	-0.42173100
H	-0.29361500	-3.37228000	-1.13851700
H	0.34726700	-1.19948300	-1.92536600
H	-1.28986400	-0.49619100	-1.54101600
H	1.14957500	3.70920200	-0.75505000
H	1.69555700	2.80461800	0.65511400
H	1.52546700	1.64092000	-2.16718800
H	2.98061200	2.35792500	-1.47922100
H	2.09336700	-0.44583300	-2.48735500
H	3.76813700	0.01977400	-2.15432100
H	4.30704400	1.08243900	-0.02553200
H	3.03531900	1.28811900	1.19186000
H	-0.59576200	1.80835600	-2.09719700
H	-0.99178100	3.44345700	-1.53906200
H	-0.75060200	3.96449100	0.88607400

H	-0.06422500	2.71668900	1.94228600
H	-4.16341500	-2.34350400	0.28557700
H	-3.04509100	-1.01658100	0.04215400
H	-4.86749500	-0.91083400	-1.65504400
H	-3.33648000	-1.27651200	-2.47909600
H	-4.50629200	-2.56480000	-2.18435400
C	-1.62713800	-2.86247200	1.79082300
H	-0.88157700	-3.63742300	1.64638400
H	-2.63654100	-3.20971900	1.97650000
C	-1.23889600	-1.60288800	2.18827700
H	-1.99851900	-0.88112500	2.48464700
C	0.12697000	-1.18955500	2.24755800
H	0.85245300	-1.95831400	1.96943600
C	0.61040100	0.03222300	2.63530300
H	-0.06302300	0.80172100	3.00012700
H	1.67122400	0.20587900	2.77063200
C	3.76275700	-0.73730500	1.01690400
H	4.55210300	-0.58860700	1.76249100
H	2.89313800	-1.13678800	1.54688500
C	3.14553600	-1.80100100	-1.16346500
H	2.21578600	-2.23082100	-0.77224600
H	3.47898800	-2.44005300	-1.98866900
C	4.20304800	-1.73591100	-0.05744200
H	5.16204200	-1.41539300	-0.48818100
H	4.36636800	-2.72508200	0.38395200
C	-2.46067400	1.93935600	-1.02148300
H	-3.04232200	2.16318900	-1.92261400
H	-2.49678700	0.85647900	-0.88035700
C	-2.14159500	2.39724800	1.41080400
H	-2.11099400	1.33057700	1.66140200
H	-2.50803900	2.93033700	2.29537200
C	-3.06428500	2.61885900	0.20940900
H	-4.06545100	2.22225800	0.40912700
H	-3.17517400	3.69714400	0.02725600

1,2-insertion transition state, DiPip as ligand (anti-allyl, cis-butadiene)

C	2.55256300	-1.87994000	-0.52795500
C	1.70849200	-1.21087100	-1.41165200
C	0.32115900	-1.34201200	-1.52284900
Li	-0.40814400	0.10076200	-0.07872000

C	4.04703100	-1.70622400	-0.55075600
C	4.79212800	-2.78554900	-1.35703600
H	2.18666500	-2.82256600	-0.12381900
H	2.17187600	-0.42266200	-2.01373100
H	-0.17598400	-0.91241400	-2.39322900
H	-0.15968400	-2.21538400	-1.08166900
H	4.29024200	-0.71697400	-0.96541200
H	4.44927300	-1.70881600	0.47596500
H	5.87968000	-2.64105900	-1.31831100
H	4.57086500	-3.78364800	-0.96118500
H	4.47881900	-2.77143600	-2.40661500
C	2.01333000	-0.94467300	1.57338800
H	2.53921500	-1.82667200	1.92198100
H	2.64044700	-0.08212100	1.38220000
C	0.67116500	-0.79153000	1.84974800
H	0.25746000	0.21912000	1.87643400
C	-0.20769900	-1.85778000	2.28473200
H	-1.14957400	-1.53308900	2.72906400
C	0.01083800	-3.19080400	2.20334000
H	0.90903500	-3.59988400	1.75137900
H	-0.71142100	-3.90098900	2.59226400
C	-1.40734300	2.56896300	-0.77720600
C	-2.54299300	1.89552600	-0.01209100
N	-2.53469700	0.42920300	-0.17471800
N	-0.08101200	2.23535100	-0.22075900
C	-3.31802800	-0.19757700	0.91509600
C	-3.11403600	0.06908900	-1.49280200
C	0.16499300	3.04412700	0.99773500
C	0.96585200	2.50986500	-1.23336800
H	-1.56440400	3.66102800	-0.78284000
H	-1.42437400	2.24617400	-1.82206700
H	-2.45126700	2.11714700	1.05513600
H	-3.50752500	2.32026500	-0.33920600
H	-2.83613100	0.06411400	1.86328400
H	-4.33662100	0.23368000	0.93459300
H	-4.11633400	0.52984100	-1.57823100
H	-2.48904000	0.50449500	-2.27680400
H	-0.59976100	2.79826200	1.73966000
H	0.04102500	4.11421700	0.74588800
H	0.89106700	3.56156600	-1.56797300
H	0.76389400	1.87148100	-2.09924000

C	-3.23283500	-1.43875800	-1.70719800
H	-3.70722400	-1.61009400	-2.68027800
H	-2.23435800	-1.88040200	-1.75209200
C	-3.41012500	-1.71464400	0.76420300
H	-2.40781900	-2.14798000	0.83762600
H	-3.99682200	-2.11344200	1.59977000
C	-4.03526900	-2.09286300	-0.58027800
H	-5.07885900	-1.74859700	-0.61687500
H	-4.05166800	-3.18099100	-0.70304900
C	1.55407400	2.82788100	1.59599300
H	1.66641000	3.50124300	2.45337600
H	1.63635900	1.80847900	1.98258900
C	2.36855300	2.24177800	-0.69480800
H	2.46010000	1.17792300	-0.45882900
H	3.09584000	2.45898100	-1.48512600
C	2.64876500	3.07887100	0.55552600
H	3.63303400	2.83434600	0.96907800
H	2.66827500	4.14544100	0.29021400

1,4-insertion transition state, glyme as ligand (syn-allyl, trans-butadiene)

C	3.61830700	0.13924100	0.18595700
C	2.63444700	-0.67377300	-0.25697100
C	1.22011500	-0.58117600	0.06319800
Li	-0.80712200	-0.17953600	-0.15480300
C	5.05665100	0.06626400	-0.24519200
C	6.01493900	-0.28556300	0.90627700
H	3.37939100	0.89013300	0.94312800
H	2.90667800	-1.41860600	-1.00955100
H	0.71029000	-1.55348100	-0.00760500
H	1.02095700	-0.10604000	1.03234300
H	5.15773200	-0.67691500	-1.04683400
H	5.37026900	1.02897900	-0.67653100
H	7.05821700	-0.29815400	0.56906000
H	5.93428400	0.44589800	1.71907700
H	5.77483800	-1.26999400	1.32242100
C	0.64533500	0.88964100	-1.45181200
H	1.14976600	0.31846700	-2.22440100
H	1.31103900	1.57897000	-0.93530900
C	-0.69274200	1.27600700	-1.67868600
H	-1.26819800	0.75444000	-2.44430200

C	-1.35930800	2.30267100	-0.93087700
H	-0.71684700	2.85754700	-0.23901200
C	-2.67354400	2.66220000	-0.97752300
H	-3.37015800	2.17507900	-1.65664800
H	-3.04874100	3.50616600	-0.40792400
C	-3.06797200	-1.67793600	0.52638200
H	-4.06578000	-1.96316900	0.16571900
H	-2.69714200	-2.45484000	1.20994600
C	-3.12960500	-0.33673200	1.22624000
H	-3.74202700	-0.42011000	2.13449900
H	-3.55037500	0.43835400	0.57030400
C	-1.69736900	1.19334600	2.37140200
H	-2.16866100	2.04020300	1.86239500
H	-0.63538200	1.39420900	2.51883800
H	-2.17534400	1.01780500	3.34313500
C	-1.98605000	-2.72513000	-1.33754300
H	-1.57763800	-3.53248800	-0.71601000
H	-1.28031600	-2.48318400	-2.13321500
H	-2.93845600	-3.04583900	-1.77740700
O	-1.78558500	0.01571800	1.56428100
O	-2.16644600	-1.53811600	-0.57138300

1,4-insertion transition state, glyme as ligand (syn-allyl, cis-butadiene)

C	3.05602600	-0.36490000	-0.61827200
C	1.80855500	0.13423800	-0.80119200
C	0.67579800	-0.55098300	-1.39303900
Li	-0.88219900	-0.29890400	0.10807800
C	4.17349700	0.35989700	0.07985400
C	5.34667400	0.71043900	-0.85294300
H	3.29872700	-1.34316900	-1.03819700
H	1.61137000	1.12160300	-0.37331000
H	-0.10985100	0.10322800	-1.78762200
H	0.92634300	-1.31297400	-2.12818900
H	3.78078600	1.28051300	0.53261200
H	4.56148900	-0.24898800	0.91027600
H	6.15775200	1.20862900	-0.30794800
H	5.75939800	-0.19352200	-1.31592100
H	5.01432900	1.37217700	-1.66024200
C	0.14213500	-2.31984900	-0.05365800
H	1.20227800	-2.23709700	0.17701600

H	-0.09257300	-2.97441900	-0.88785900
C	-0.79032500	-2.22422900	0.98675400
H	-1.76758300	-2.68832800	0.87646600
C	-0.53961900	-1.45824600	2.17901300
H	-1.31319500	-1.50382400	2.94652600
C	0.53300100	-0.64342300	2.41131100
H	1.35658200	-0.55664900	1.70787900
H	0.62979800	-0.11852300	3.35657900
C	-3.38883500	0.91150700	-0.55184900
H	-4.12962700	1.20626900	-1.30855900
H	-3.91698200	0.60692200	0.36359600
C	-2.44876000	2.06375700	-0.26443900
H	-2.99844000	2.88829100	0.21082600
H	-1.98989900	2.43144800	-1.19356500
C	-0.53060900	2.55832800	1.07782600
H	-0.00601700	3.03127100	0.23775200
H	0.18276700	2.03822600	1.71727700
H	-1.06613900	3.32208600	1.65556500
C	-3.32445700	-1.32328800	-1.39707900
H	-3.89056000	-1.71563100	-0.54254900
H	-2.59601300	-2.06626700	-1.72191500
H	-4.01211300	-1.09260500	-2.22068300
O	-1.44145000	1.56546900	0.60838800
O	-2.58661400	-0.16314900	-1.02635800

1,4-insertion transition state, glyme as ligand (anti-allyl, trans-butadiene)

C	3.66151300	0.79298600	0.16244000
C	2.65776900	1.69973500	0.09142900
C	1.25102600	1.40285800	-0.13003700
C	3.48695500	-0.68289100	-0.09466400
C	3.61029900	-1.06345400	-1.58304400
H	4.66917500	1.14252700	0.37735400
H	2.90843500	2.73870200	0.30647600
H	0.66454600	2.26754800	-0.45949400
H	1.10644200	0.55640100	-0.81326000
H	4.23061400	-1.24889500	0.48011900
H	2.50596600	-1.00967200	0.27634700
H	3.47439200	-2.14177600	-1.73549400
H	2.86202100	-0.53291500	-2.18149700
H	4.59613300	-0.78939500	-1.97345900

C	0.65639200	0.98170900	1.91897100
H	1.53832800	0.35499400	2.03371900
H	0.84117000	2.01991000	2.17547400
C	-0.60465300	0.43353600	2.24539800
H	-1.44376800	1.10635500	2.42558800
C	-0.85371500	-0.97737100	2.30852300
H	0.03944500	-1.60419900	2.21484000
C	-2.04516400	-1.62201100	2.46687300
H	-2.97515600	-1.07141100	2.59144900
H	-2.09305200	-2.70118100	2.56979100
Li	-0.58652000	0.43400300	0.14448900
C	-2.31208300	-1.13790700	-1.22443000
H	-2.60109500	-1.85493300	-2.00492700
H	-2.76913800	-1.43041600	-0.26846600
C	-2.73288100	0.25851200	-1.63124800
H	-3.82836400	0.32508600	-1.67993600
H	-2.31244300	0.51951100	-2.61272400
C	-2.52624700	2.52662100	-0.88752400
H	-2.09052600	2.85619200	-1.83944100
H	-2.08822400	3.09726300	-0.06765600
H	-3.61164900	2.68438600	-0.90486300
C	-0.32097900	-2.40566800	-0.84752400
H	-0.75226900	-2.85992900	0.05042900
H	0.75081400	-2.25724000	-0.71089400
H	-0.49330200	-3.04883100	-1.71932800
O	-2.22705200	1.15565600	-0.64220300
O	-0.89024000	-1.11315900	-1.07462100

1,4-insertion transition state, glyme as ligand (anti-allyl, cis-butadiene)

C	3.09149600	0.84691700	-0.15933500
C	1.78658400	0.82855300	-0.53595800
C	0.99239400	-0.30636500	-0.97189700
C	4.07196400	-0.29054600	-0.27183400
C	5.23426200	0.03157200	-1.22863600
H	3.50555500	1.78881600	0.20061700
H	1.24367900	1.76809300	-0.41484300
H	0.12016300	-0.04326700	-1.58118500
H	1.53747300	-1.11389400	-1.45481000
H	3.56480500	-1.20005900	-0.61193000
H	4.49071000	-0.52834500	0.71682800

H	4.86096500	0.21626000	-2.24174300
H	5.95813400	-0.79110900	-1.27166900
H	5.76832600	0.93222500	-0.90368500
C	0.77436800	-1.72831200	0.79408900
H	1.69719100	-1.24100800	1.09616300
H	0.90807100	-2.61685000	0.18462100
C	-0.32589000	-1.68468200	1.66059000
H	-1.08730800	-2.45866300	1.60167500
C	-0.54052900	-0.59529500	2.57547900
H	-1.39722300	-0.69457800	3.24316100
C	0.18064500	0.56449900	2.64207800
H	1.06025800	0.73613100	2.02721500
H	-0.06337100	1.32177200	3.38053400
Li	-0.81421900	-0.19590200	0.23848200
C	-3.39278600	-0.08880500	-1.00192900
H	-4.03060600	-0.26863700	-1.87891200
H	-3.97832300	-0.28013600	-0.09073500
C	-2.87845700	1.33570600	-1.01343100
H	-3.71345500	2.03827500	-0.88277500
H	-2.37223900	1.55805000	-1.96387200
C	-1.45698200	2.76960500	0.27080500
H	-0.93313100	3.13045300	-0.62354700
H	-0.76244900	2.70418700	1.10849700
H	-2.27982800	3.45226100	0.51736300
C	-2.55848600	-2.32699200	-1.07526600
H	-3.14224200	-2.62734500	-0.19565700
H	-1.60654300	-2.85797700	-1.07767400
H	-3.11852200	-2.56494600	-1.98859200
O	-1.95611700	1.44894000	0.06412200
O	-2.25124900	-0.93733100	-1.02899900

1,2-insertion transition state, glyme as ligand (syn-allyl, trans-butadiene)

C	2.91683500	-0.02607800	0.59510500
C	1.79513800	-0.83974200	0.51582700
C	0.59263300	-0.72127300	1.22617900
Li	-0.97270600	0.24292700	0.08627800
C	4.20250300	-0.34560900	-0.11935500
C	5.23269500	-1.08771000	0.75156100
H	3.00199600	0.62316200	1.46653200
H	1.82102900	-1.60247600	-0.27091800

H	-0.08702200	-1.57501700	1.23638700
H	0.57871100	-0.12531700	2.13966500
H	3.97915800	-0.95401400	-1.00785600
H	4.67442800	0.57595800	-0.49706700
H	6.16699200	-1.27079200	0.20488400
H	5.47565200	-0.50223700	1.64615000
H	4.83417200	-2.05109300	1.08778700
C	-1.48734900	2.17618600	-1.18665700
H	-1.83106800	2.85172800	-0.40571500
H	-2.21596200	1.85441200	-1.92272200
C	-0.16082300	1.87068400	-1.32110500
H	0.12067500	1.23600200	-2.16604900
C	0.92270500	2.27239800	-0.47732100
H	0.69235000	2.92508200	0.36434000
C	2.22102800	1.86948400	-0.68504900
H	2.48703200	1.32868700	-1.58804300
H	3.04150900	2.35172000	-0.16842300
C	-2.89818400	-1.75564000	-0.27752800
H	-3.58912200	-2.31819100	-0.92151700
H	-2.50087100	-2.43113100	0.49362800
C	-3.62045700	-0.59319800	0.36858900
H	-4.44065700	-0.96563700	0.99827000
H	-4.03289000	0.07903900	-0.39720700
C	-3.21613300	1.21598700	1.87034300
H	-3.64547500	1.94862900	1.17538700
H	-2.39634500	1.67477700	2.42469000
H	-3.98788600	0.87638500	2.57259300
C	-0.99293100	-2.20953200	-1.63851500
H	-0.53611100	-2.84316600	-0.86855700
H	-0.20851500	-1.68026700	-2.17986300
H	-1.57093000	-2.82911700	-2.33583700
O	-2.66693200	0.10856800	1.16245100
O	-1.82790400	-1.21627400	-1.04642800

1,2-insertion transition state, glyme as ligand (syn-allyl, cis-butadiene)

C	2.24239200	-0.21162100	-0.29223400
C	1.71914600	-0.03138400	-1.58993000
C	0.53645600	-0.50833400	-2.12100700
Li	-0.47900700	0.24262800	-0.18085600
C	3.69861900	0.02229300	0.01131800

C	4.59430700	-1.20876200	-0.21928200
H	1.76443400	-0.97162800	0.33354400
H	2.26652500	0.68944100	-2.20584900
H	0.23560600	-0.23715000	-3.12689900
H	0.02335800	-1.35760600	-1.67140600
H	4.06804800	0.84811600	-0.61373000
H	3.82573300	0.35353000	1.05400000
H	5.64203800	-0.99631600	0.03013800
H	4.26525500	-2.05117700	0.40088100
H	4.54717200	-1.53198900	-1.26472500
C	1.53241400	1.92823500	0.60763300
H	1.87607400	1.53022100	1.55715900
H	2.30668900	2.32523500	-0.03603800
C	0.22700900	2.36120900	0.45449200
H	-0.01829800	2.98422800	-0.40204300
C	-0.84446000	2.06978900	1.38230100
H	-1.79484500	2.55699400	1.16559300
C	-0.81057900	1.23078600	2.45276100
H	0.09570100	0.70932200	2.74924100
H	-1.67887700	1.10549400	3.09125500
C	-3.00012200	-0.93086100	-0.69489300
H	-4.09725500	-0.86086800	-0.71218100
H	-2.67073200	-1.55803200	-1.53578300
C	-2.54152300	-1.52377600	0.61870800
H	-2.94476400	-2.54001600	0.73019200
H	-2.88061700	-0.90511200	1.46093700
C	-0.56113400	-2.19561400	1.74942700
H	-0.85901800	-1.66898000	2.66354600
H	0.52313700	-2.15757900	1.64335500
H	-0.88773000	-3.24216500	1.79706800
C	-2.71839500	1.02991700	-2.02293200
H	-2.35292400	0.45176000	-2.87994700
H	-2.20217700	1.98970100	-1.99291800
H	-3.80059700	1.19093800	-2.11143300
O	-1.11568200	-1.55981100	0.59978600
O	-2.41678100	0.36287200	-0.79973200

1,2-insertion transition state, glyme as ligand (anti-allyl, trans-butadiene)

C	2.94721400	-0.24037200	-0.81383300
C	1.91540800	-0.23556800	-1.74910300

C	0.60507000	-0.70152200	-1.58876600
Li	-0.72400700	0.43890800	-0.28457000
C	2.85673000	-1.03442700	0.46102000
C	3.04882500	-2.55162600	0.28090700
H	3.93973000	0.04659300	-1.15313400
H	2.12387000	0.29709900	-2.68001000
H	-0.03851800	-0.71947900	-2.46677900
H	0.39618100	-1.47886500	-0.85297400
H	3.59821200	-0.66748200	1.18456800
H	1.87205400	-0.85298200	0.91767500
H	2.92750700	-3.08955700	1.23068500
H	2.32500800	-2.95182300	-0.43595400
H	4.05028400	-2.77131300	-0.10524600
C	-1.09900400	2.62112500	0.51897700
H	-1.31684600	2.36471700	1.55368200
H	-1.90785700	3.05222700	-0.06061800
C	0.17241700	2.53700300	0.01837300
H	0.33036400	2.86484500	-1.01140700
C	1.34092500	2.04909100	0.68800100
H	1.23660200	1.75093500	1.73064400
C	2.57017700	1.93429800	0.07876400
H	2.73450800	2.37464300	-0.89863500
H	3.46018100	1.74622700	0.66750700
C	-3.03170900	-1.16742800	-0.13684000
H	-4.12222300	-1.28052500	-0.21767900
H	-2.55050400	-2.09508700	-0.47832300
C	-2.64844600	-0.87171500	1.29665300
H	-2.93421800	-1.71577500	1.94002300
H	-3.15520300	0.03693400	1.65221700
C	-0.71591600	-0.48968400	2.64003600
H	-1.14668400	0.40669300	3.10434000
H	0.36160700	-0.36562400	2.53440800
H	-0.92817300	-1.36602100	3.26519400
C	-2.89421300	-0.21166600	-2.31533900
H	-2.43088600	-1.11549300	-2.72969600
H	-2.48985200	0.66640700	-2.81988600
H	-3.98117300	-0.25250700	-2.46158000
O	-1.23749800	-0.68084300	1.32733000
O	-2.58585500	-0.07247700	-0.93088200

1,2-insertion transition state, glyme as ligand (anti-allyl, cis-butadiene)

C	-2.81309600	-0.25697000	-0.70269400
C	-1.84715500	-0.57548400	-1.65685900
C	-0.60121300	0.01451400	-1.87521600
C	-2.75985500	1.00253500	0.12135600
C	-3.30321300	2.24941300	-0.60168400
H	-3.79130500	-0.72033600	-0.80530500
H	-2.04828700	-1.48367500	-2.22952100
H	-0.00084700	-0.32346100	-2.71600300
H	-0.42355000	1.04815200	-1.57444300
H	-1.72282400	1.20077300	0.42663000
H	-3.32047800	0.86415500	1.05731400
H	-3.24059600	3.14623200	0.02963700
H	-2.74191000	2.43430500	-1.52322400
H	-4.35332200	2.10517000	-0.87830800
C	-2.24169800	-2.04151800	0.87984500
H	-2.60596300	-1.33051000	1.61407300
H	-2.99465700	-2.64681900	0.39108300
C	-0.93190400	-2.46354100	0.89835900
H	-0.65578600	-3.32434000	0.29394200
C	0.12629200	-1.84429400	1.64908700
H	1.06094000	-2.40627600	1.68611400
C	0.12305400	-0.63246500	2.28298500
H	-0.76336700	-0.00305300	2.31609600
H	0.97423800	-0.31815400	2.87843600
Li	0.51130400	-0.20803700	-0.00422600
C	3.14340200	0.41453000	-0.73972700
H	4.22285500	0.20747800	-0.71926100
H	2.86966400	0.78568300	-1.73769800
C	2.79078100	1.43826100	0.31673600
H	3.32355900	2.37955400	0.12104300
H	3.06951600	1.07115700	1.31507500
C	0.90789800	2.60984900	1.18831500
H	1.10722000	2.28601200	2.21737300
H	-0.16831000	2.69649200	1.03636100
H	1.38273600	3.58231000	1.00668400
C	2.59151800	-1.81377800	-1.39314000
H	2.29250700	-1.48573300	-2.39583700
H	1.95076300	-2.63861000	-1.08095400
H	3.64043400	-2.13688500	-1.40119200
O	1.38281000	1.64437800	0.25372300

O	2.40393900	-0.76585500	-0.44367300
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1,4-insertion transition state, THF as ligand (syn-allyl, trans-butadiene)

C	3.49143100	-1.56555800	-0.30981100
C	2.55108200	-0.59814900	-0.36111800
C	1.11536000	-0.78260300	-0.53544500
C	4.94863500	-1.33696200	-0.01922100
C	5.86585800	-1.72285300	-1.19276800
H	3.19733000	-2.59507000	-0.52526800
H	2.88290500	0.42215600	-0.14619800
H	0.66317500	0.07737100	-1.04829600
H	0.84376100	-1.69744800	-1.06572800
H	5.10646300	-0.28109500	0.23837600
H	5.25179700	-1.91827500	0.86463000
H	6.92253800	-1.57716600	-0.93930100
H	5.72851200	-2.77572300	-1.46544600
H	5.63670800	-1.11971200	-2.07801300
C	0.52840600	-1.38835500	1.40750100
H	0.73653400	-2.40724400	1.08657300
H	1.39748300	-0.93278000	1.87336900
C	-0.74015200	-1.12652800	1.98431300
H	-0.84076700	-0.28695800	2.67443900
C	-1.89283900	-1.94618700	1.75122700
H	-1.71237800	-2.81616600	1.11096400
C	-3.16070400	-1.78557000	2.22220500
H	-3.42118200	-0.96358700	2.88591000
H	-3.93669900	-2.51472500	2.01427800
Li	-0.68951000	0.13964100	0.31163300
C	-0.24959700	2.87420800	-0.53676000
C	0.80240600	2.30955800	1.49982900
C	1.23942900	3.13521300	-0.73449600
H	-0.79939500	3.80202500	-0.32573700
H	-0.73579900	2.34666300	-1.36010500
C	1.73586300	3.25357200	0.71832600
H	1.27772300	1.35840700	1.74881100
H	0.41086500	2.76316600	2.41543800
H	1.70472500	2.28156200	-1.23667500
H	1.43571700	4.03394100	-1.32531700
H	2.78538000	2.97008200	0.82870500
H	1.62691500	4.28288000	1.07451400

C	-3.36398500	0.63867000	-0.46993100
C	-2.32726000	-1.06527300	-1.77374500
C	-4.44263800	-0.07386400	-1.28126600
H	-3.35530000	1.72476900	-0.59367100
H	-3.43311100	0.37918300	0.59165800
C	-3.79058100	-1.43969000	-1.54673000
H	-1.62413000	-1.83267900	-1.44158000
H	-2.11851800	-0.81808800	-2.82126700
H	-5.38249700	-0.15194400	-0.72875200
H	-4.63573100	0.45495000	-2.22162000
H	-3.88064800	-2.07117700	-0.65878200
H	-4.22068100	-1.96462900	-2.40394000
O	-0.31424400	2.01154900	0.61833200
O	-2.09918500	0.12977600	-0.97952300

1,4-insertion transition state, THF as ligand (syn-allyl, cis-butadiene)

C	3.11807600	-1.41383000	-0.68375300
C	2.03331400	-0.60803900	-0.79261100
C	0.72739400	-0.96856800	-1.30925400
C	4.42020400	-1.00718000	-0.05054700
C	5.58574100	-0.92826500	-1.05292000
H	3.07956400	-2.41463300	-1.11843700
H	2.12155300	0.38591700	-0.34934000
H	0.12994100	-0.12635500	-1.67787100
H	0.72422400	-1.77270500	-2.04291700
H	4.29505900	-0.03170700	0.43929700
H	4.69442500	-1.71626900	0.74478600
H	6.52598500	-0.66084400	-0.55539400
H	5.73362600	-1.89178100	-1.55445300
H	5.37928300	-0.18174000	-1.82770600
C	-0.15727100	-2.47360900	0.13110600
H	0.89681000	-2.68123700	0.30441700
H	-0.60945000	-3.06474100	-0.65990600
C	-0.96406900	-2.11292500	1.21671100
H	-2.03598000	-2.28694800	1.16628200
C	-0.44527500	-1.45903400	2.38853800
H	-1.15772000	-1.30046300	3.19963300
C	0.82500700	-0.98967400	2.56619400
H	1.59855200	-1.12081400	1.81443800
H	1.11943700	-0.53986500	3.50917600

Li	-0.61932000	-0.20938200	0.24914600
C	-0.46741000	2.63979900	-0.57097400
C	0.69251000	2.30794300	1.39324800
C	0.95678800	3.08404300	-0.90926200
H	-1.08743400	3.48707900	-0.24103200
H	-0.98692600	2.10550200	-1.36652000
C	1.66787700	3.07124500	0.46903000
H	1.13939200	1.48573400	1.95236900
H	0.18751700	2.98637800	2.09342500
H	1.41807900	2.36046500	-1.58655000
H	0.98072300	4.06568000	-1.39012100
H	2.63630500	2.56897300	0.40785400
H	1.84301000	4.08345500	0.84406700
C	-3.40180900	0.57009400	0.31160700
C	-2.92908300	-0.83842500	-1.54199300
C	-4.71779500	-0.01088000	-0.20940500
H	-3.38256700	1.66246700	0.34667500
H	-3.14903500	0.17962600	1.30465400
C	-4.24983000	-1.28924100	-0.92257900
H	-2.19413700	-1.63607500	-1.66027100
H	-3.08308100	-0.34567800	-2.51056000
H	-5.43241700	-0.20149400	0.59548300
H	-5.18468000	0.67532900	-0.92471800
H	-4.07458500	-2.09056000	-0.19738200
H	-4.96018600	-1.65113800	-1.67058900
O	-0.30352300	1.72521400	0.52640200
O	-2.38067100	0.13176800	-0.61828400

1,4-insertion transition state, THF as ligand (anti-allyl, trans-butadiene)

C	-3.19536200	-2.38192000	-0.07850400
C	-1.99760100	-2.84528300	-0.51001700
C	-0.78497100	-2.06480900	-0.71355600
C	-3.50749700	-0.92752200	0.15982700
C	-4.17429000	-0.24385500	-1.04966300
H	-4.00767800	-3.09052900	0.07246800
H	-1.90331800	-3.92483700	-0.63298000
H	-0.03835600	-2.55438200	-1.34131600
H	-1.00307000	-1.06093900	-1.09737200
H	-4.17036600	-0.82861400	1.03008100
H	-2.58682900	-0.38762800	0.40841300

H	-4.37868300	0.81656800	-0.85227900
H	-3.53108100	-0.31441600	-1.93349300
H	-5.12451400	-0.72865200	-1.29840000
C	0.08886100	-2.26330500	1.28152800
H	-0.89537100	-2.15839700	1.73501400
H	0.32613500	-3.28666700	1.01090200
C	1.13468100	-1.44977600	1.77153800
H	2.16420200	-1.72208200	1.53777800
C	0.92372600	-0.29071500	2.58788700
H	-0.11753900	-0.11882900	2.87785800
C	1.84475000	0.60344000	3.04887500
H	2.90549600	0.48941400	2.83624600
H	1.56184100	1.40998800	3.71672300
Li	0.38232300	-0.40671700	0.04739800
C	-1.12865800	2.04934900	1.08802400
C	-0.88578000	1.87540900	-1.27310900
C	-1.93444700	3.16676600	0.42120300
H	-0.28780900	2.42378700	1.67956700
H	-1.73778100	1.39304600	1.71469300
C	-1.23206300	3.32237700	-0.93679400
H	-1.73753100	1.35238000	-1.72444300
H	-0.00964500	1.75284600	-1.91354100
H	-2.97339200	2.85322700	0.27428300
H	-1.93569100	4.08427200	1.01519400
H	-1.86335100	3.78786800	-1.69822500
H	-0.31912100	3.91916600	-0.83238600
O	-0.58162900	1.25925500	0.00023300
C	2.64623400	-1.12303800	-1.63256700
C	2.73118200	0.98791800	-0.53187100
C	4.10444700	-0.66954800	-1.55020200
H	2.30516600	-1.34074000	-2.64783900
H	2.45560900	-1.99493600	-0.99705600
C	4.07830900	0.29493600	-0.35424900
H	2.28003400	1.31606700	0.40776400
H	2.79778300	1.83603900	-1.22536500
H	4.78960200	-1.51003000	-1.41255900
H	4.39476200	-0.13830000	-2.46346000
H	4.09182600	-0.25980500	0.58923900
H	4.91243100	1.00149000	-0.35049900
O	1.85914900	-0.01410200	-1.12489800

1,4-insertion transition state, THF as ligand (anti-allyl, cis-butadiene)

C	3.54926900	-0.09303900	-0.12882100
C	2.26585700	0.15264200	-0.50212400
C	1.26332600	-0.79383500	-0.95551100
C	4.28792600	-1.39760800	-0.26989600
C	5.49170600	-1.28961900	-1.22363900
H	4.13850600	0.74111900	0.25244400
H	1.91623700	1.17653400	-0.35964900
H	0.46275400	-0.35481600	-1.56114500
H	1.63692800	-1.69084300	-1.44357000
H	3.61199700	-2.18199300	-0.62786500
H	4.65087100	-1.73543800	0.71174000
H	5.16273400	-1.01288200	-2.23116800
H	6.04006800	-2.23727800	-1.28723300
H	6.19204000	-0.51871700	-0.88110600
C	0.71611800	-2.14886600	0.78550000
H	1.72967000	-1.91236100	1.09800300
H	0.63165700	-3.01801300	0.14073700
C	-0.33863000	-1.87993300	1.66413200
H	-1.27160400	-2.42812700	1.56026500
C	-0.27459300	-0.84914400	2.66693000
H	-1.12344000	-0.79776400	3.35070400
C	0.71151500	0.08286900	2.81732600
H	1.59222300	0.10101800	2.18012900
H	0.66894600	0.80846200	3.62313400
Li	-0.43354800	-0.18416700	0.30808500
C	-0.89573100	2.32237800	-1.18515300
C	-0.18371100	2.77818200	1.03585600
C	-0.09999000	3.62418600	-1.19425200
H	-1.96885200	2.50097500	-1.33461000
H	-0.55706000	1.58832500	-1.91835400
C	-0.25485900	4.09445800	0.25975800
H	0.84283300	2.50709100	1.29994600
H	-0.78978800	2.76297600	1.94426900
H	0.95174100	3.42183900	-1.42315300
H	-0.48019500	4.34174800	-1.92633600
H	0.52085500	4.79843800	0.57212300
H	-1.22907500	4.57589900	0.40199800
C	-3.29938800	-0.27519300	0.01537900
C	-2.21791100	-1.84681000	-1.39950200
C	-4.33318400	-1.29999000	-0.45328800

H	-3.57337700	0.76159700	-0.19630300
H	-3.08766000	-0.37376800	1.08720500
C	-3.45285400	-2.51230500	-0.79510300
H	-1.29157500	-2.40358600	-1.24737400
H	-2.34603400	-1.64959200	-2.47123900
H	-5.08299100	-1.51207900	0.31339500
H	-4.85209200	-0.94036800	-1.34884200
H	-3.18324400	-3.05761800	0.11531400
H	-3.93018700	-3.21204200	-1.48621000
O	-0.69900600	1.76321000	0.13474700
O	-2.08742600	-0.57652100	-0.71687900

1,2-insertion transition state, THF as ligand (syn-allyl, trans-butadiene)

C	2.94632200	-1.25033100	-0.59956900
C	2.04974500	-0.23373800	-0.91534000
C	0.76320000	-0.37088200	-1.44202700
C	4.35390000	-0.97112400	-0.14443500
C	5.39118700	-0.96222200	-1.28210400
H	2.78625000	-2.21375500	-1.08281600
H	2.35134400	0.77525800	-0.61311300
H	0.26305900	0.50516900	-1.85437600
H	0.48961000	-1.31818900	-1.90589500
H	4.37941400	-0.00034600	0.37240900
H	4.67025800	-1.71686000	0.60258300
H	6.40684000	-0.78921800	-0.90277200
H	5.38929000	-1.92118900	-1.81351900
H	5.15786100	-0.18115900	-2.01399400
C	2.02245700	-2.16667700	1.35884000
H	2.57086100	-1.44975300	1.96349400
H	2.58076400	-3.04587500	1.06186800
C	0.64450800	-2.19041900	1.40811200
H	0.10240000	-2.99536300	0.91308400
C	-0.11830800	-1.20165100	2.10464800
H	0.47619700	-0.44725600	2.62582000
C	-1.47737200	-1.08874800	2.19947500
H	-2.13591900	-1.83237900	1.75699000
H	-1.93620700	-0.32135500	2.81349700
Li	-0.74099900	-0.04238800	0.14992100
C	-0.85706800	2.82031400	-0.44150900
C	0.55427000	2.26791000	1.37513000

C	0.51281100	3.41916900	-0.73919800
H	-1.56449400	3.58527500	-0.09165000
H	-1.30553200	2.27169600	-1.27184900
C	1.12528600	3.50727300	0.66889600
H	1.25141100	1.42620500	1.35531100
H	0.25571400	2.46208900	2.40985900
H	1.08993200	2.73825500	-1.37215000
H	0.44884900	4.38948500	-1.23913400
H	2.21813100	3.50296100	0.65970400
H	0.79484900	4.42337300	1.16988200
C	-3.65076000	0.27399700	-0.15124000
C	-2.75797900	-1.12297300	-1.75783800
C	-4.46509100	-1.03628000	-0.05131300
H	-4.18344700	1.03499500	-0.73674400
H	-3.36469200	0.69720800	0.81226800
C	-3.69899000	-2.02990800	-0.96278600
H	-1.82184900	-1.58911900	-2.06578200
H	-3.25596100	-0.69290600	-2.63876400
H	-4.51277700	-1.39877800	0.97793900
H	-5.49069700	-0.88046000	-0.39695800
H	-3.11455500	-2.73195400	-0.36159600
H	-4.36239500	-2.60913600	-1.61039300
O	-0.62429200	1.87303400	0.62315400
O	-2.43073700	-0.06453700	-0.84058300

1,2-insertion transition state, THF as ligand (syn-allyl, cis-butadiene)

C	-2.62544700	-1.27097000	0.42190200
C	-1.97392000	-0.25058500	1.12040600
C	-0.73859500	-0.31184900	1.76453900
C	-4.01705600	-1.10286200	-0.12600800
C	-5.13258600	-1.56271200	0.83065200
H	-2.33413800	-2.29015500	0.67326500
H	-2.44663600	0.73693700	1.06638500
H	-0.42669500	0.50999700	2.40824400
H	-0.29143200	-1.28358800	1.97372600
H	-4.17958600	-0.04477400	-0.38217400
H	-4.12591500	-1.66027800	-1.07069700
H	-6.12637200	-1.45280600	0.37693400
H	-4.99916100	-2.61735800	1.09834500
H	-5.11088200	-0.98294900	1.75990900

C	-1.40523000	-1.53148900	-1.58796400
H	-1.84491200	-2.52126200	-1.53051200
H	-2.01509100	-0.78705100	-2.08791900
C	-0.03400700	-1.38075800	-1.53237900
H	0.40000300	-0.47963300	-1.97259600
C	0.89607800	-2.38649200	-1.06102100
H	1.94064800	-2.20885900	-1.32322700
C	0.62196600	-3.50434700	-0.34599000
H	-0.38471500	-3.74384200	-0.01729400
H	1.40587300	-4.20711400	-0.08286200
Li	0.48848300	0.23128600	0.04251500
C	0.50928800	3.06500900	0.18188300
C	-1.11718800	2.22886600	-1.29919600
H	0.97132600	3.88795000	-0.38183200
H	-0.98680000	2.52445100	-2.34534800
C	3.35466000	0.51328700	-0.61328600
C	2.87435000	-0.76413300	1.34080800
C	4.66436900	-0.06520800	-0.08129600
H	3.37399500	1.59451200	-0.77187500
H	3.04614000	0.02439500	-1.54595800
C	4.17331200	-1.27941300	0.72286500
H	2.10974500	-1.53459000	1.45594400
H	3.04272000	-0.26503700	2.30180600
H	5.35735500	-0.32973100	-0.88430400
H	5.16124300	0.65615800	0.57697200
H	3.96544100	-2.12169200	0.05508200
H	4.88789900	-1.61226100	1.48003600
O	0.19472900	1.98612600	-0.72175400
O	2.36846200	0.23168400	0.40690000
H	1.22746400	2.67828900	0.90823200
H	-1.66151500	1.28424000	-1.25668200
C	-0.83836700	3.46950100	0.76903300
H	-1.12373000	2.76518200	1.55550500
H	-0.83045200	4.47840900	1.19023300
C	-1.77285800	3.33648300	-0.44927600
H	-1.81112000	4.27729400	-1.00714000
H	-2.79428900	3.07486800	-0.16294100

1,2-insertion transition state, THF as ligand (anti-allyl, trans-butadiene)

C	-3.10455300	-1.17501700	-1.17298800
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C	-1.86031600	-1.46566700	-1.73675600
C	-0.68885700	-0.71083700	-1.66374500
C	-3.42457000	0.19621500	-0.64062100
C	-3.66740200	1.26095800	-1.72593400
H	-3.94522200	-1.80052700	-1.46460700
H	-1.76679000	-2.45466600	-2.19131300
H	0.16896300	-1.03274400	-2.24937800
H	-0.75410400	0.36137300	-1.49011800
H	-4.30848500	0.14830600	0.01047700
H	-2.59531800	0.52202700	0.00434200
H	-3.83979200	2.25395500	-1.28832400
H	-2.81202000	1.32642400	-2.40627200
H	-4.54462400	1.00494500	-2.32996200
C	-2.85857300	-2.31856500	0.83276400
H	-2.68780500	-3.25349500	0.30934200
H	-3.89746300	-2.07299300	1.02245400
C	-1.86550400	-1.79386700	1.63508500
H	-2.10727000	-0.96720100	2.30178100
C	-0.52037000	-2.27830400	1.63926500
H	-0.33881200	-3.14422500	0.99796500
C	0.54661100	-1.78419300	2.34178800
H	0.43454100	-0.95368500	3.03509900
H	1.50939000	-2.28325800	2.32168400
Li	0.45046700	-0.66049700	0.26228800
C	3.33915900	-0.31208400	0.66833400
C	2.90308400	-0.85514100	-1.60167900
C	4.45836300	0.27833100	-0.18479200
H	3.68167900	-1.18604500	1.23664200
H	2.86538100	0.39437200	1.35229900
C	4.40674200	-0.62053000	-1.43016900
H	2.44088700	-0.09509900	-2.24250300
H	2.65507700	-1.84317700	-1.99821600
H	4.22834800	1.31651400	-0.45027200
H	5.42683700	0.26029600	0.32204800
H	4.85773100	-0.16434600	-2.31526400
H	4.92297000	-1.56670400	-1.23474500
C	-0.51776200	1.75447200	1.78320600
C	0.79331200	2.24616000	-0.11943500
C	-0.94184200	3.12958000	1.24151800
H	-0.07872100	1.80617800	2.78452200
H	-1.34148300	1.03725000	1.79140500

C	-0.46997800	3.09300400	-0.22210600
H	1.06534900	1.72946700	-1.04193900
H	1.65249000	2.84025100	0.22471300
H	-2.01917500	3.28779500	1.33371300
H	-0.43397400	3.93296600	1.78549800
H	-1.20752800	2.58970300	-0.85366000
H	-0.27959800	4.08706100	-0.63575800
O	2.33218600	-0.73776000	-0.27770400
O	0.48430000	1.24196900	0.86633900

1,2-insertion transition state, THF as ligand (anti-allyl, cis-butadiene)

C	-2.09509600	-2.39196900	-0.67769000
C	-0.83025100	-2.36364200	-1.27092500
C	-0.04642200	-1.26484600	-1.61135000
C	-2.95627200	-1.16277200	-0.54901200
C	-3.68296300	-0.75930700	-1.84562700
H	-2.61902800	-3.34489600	-0.66861600
H	-0.34370700	-3.33770200	-1.36040100
H	0.90807300	-1.42856600	-2.10365400
H	-0.51162300	-0.30395400	-1.82904100
H	-2.34004600	-0.31885400	-0.21020000
H	-3.70548800	-1.31227300	0.24151200
H	-4.28113200	0.15249300	-1.71138900
H	-2.96574600	-0.58877300	-2.65565400
H	-4.35756000	-1.55815300	-2.17183900
C	-1.36224300	-2.79084900	1.55857400
H	-2.26856100	-2.26742000	1.84707300
H	-1.47120500	-3.85110700	1.36652100
C	-0.12682400	-2.29266900	1.91773700
H	0.73823200	-2.94569200	1.82975500
C	0.12251700	-0.96784700	2.41154400
H	1.11268100	-0.81523400	2.84460300
C	-0.70053000	0.12414900	2.39796000
H	-1.71141900	0.07809300	2.00126500
H	-0.40865900	1.03997700	2.90055000
Li	0.33317400	-0.00734100	0.19303900
C	2.82955500	0.93936000	-0.96811200
C	3.08970600	-0.85990800	0.56141200
C	3.79549600	-0.07370100	-1.57677000
H	3.34773000	1.85604800	-0.65708300

H	1.99300500	1.20556500	-1.61641300
C	4.33107400	-0.79115400	-0.32871800
H	2.48925300	-1.75395900	0.36157100
H	3.31211400	-0.80848600	1.63027000
H	3.25234600	-0.77535600	-2.21775500
H	4.57910600	0.40314300	-2.17183200
H	4.73888100	-1.78267500	-0.54214700
H	5.11660600	-0.19394900	0.14775500
C	0.19679400	2.90516900	0.51536200
C	-1.39141500	2.28064900	-1.02144000
C	-1.12849200	3.48513600	1.05631800
H	0.76470000	3.65878000	-0.04703900
H	0.84255000	2.46684800	1.27656100
C	-2.21115900	2.88955900	0.11766000
H	-1.84996000	1.41619400	-1.50034000
H	-1.14543600	3.02844800	-1.78931800
H	-1.30015100	3.18479600	2.09199300
H	-1.11543000	4.57800700	1.02246500
H	-2.77328500	2.10344400	0.62857700
H	-2.92258600	3.63816200	-0.24064800
O	2.28689600	0.29990200	0.21410900
O	-0.17497600	1.84596500	-0.388827

4 TEEDA, conformation 1

C	-0.40529600	-0.98269500	-0.96490300
C	0.89567400	-0.17838400	-1.04264000
N	1.63665700	-0.11345100	0.21763500
N	-1.51664200	-0.30766300	-0.28536500
C	3.06634000	0.13474100	0.01076600
C	1.04245600	0.77306400	1.23000800
C	-2.49147300	-1.27073600	0.23715400
C	-2.14263700	0.70732000	-1.13716100
H	-0.17750200	-1.90568300	-0.42664400
H	-0.70372600	-1.27265800	-1.99272700
H	1.53084000	-0.69060500	-1.77089700
H	0.70577200	0.82473500	-1.46570500
H	3.48282700	0.46221400	0.96987100
H	3.24507700	0.96133900	-0.70325200
H	1.59138500	0.60203300	2.16426200
H	0.01363700	0.44587400	1.38545200

H	-3.42776000	-0.73829900	0.42590500
H	-2.72287500	-2.04428600	-0.52184600
H	-1.35451600	1.18584100	-1.72541000
H	-2.83158100	0.23886400	-1.86837600
C	-2.87105100	1.78740200	-0.33810100
H	-3.30144000	2.53497600	-1.01335300
H	-3.68857400	1.37634000	0.26227700
H	-2.17453500	2.28912700	0.34039900
C	-2.03601300	-1.92810000	1.53969000
H	-1.89441900	-1.17117100	2.31725500
H	-2.78642800	-2.64737400	1.88541300
H	-1.08973000	-2.46424600	1.42079800
C	1.04489600	2.27716800	0.90886900
H	0.59537700	2.83339600	1.73902700
H	2.05786400	2.66524800	0.75778100
H	0.46000200	2.50092900	0.01093300
C	3.82470000	-1.11183700	-0.44829000
H	3.69885100	-1.91979000	0.27898500
H	3.47237200	-1.47503400	-1.41914200
H	4.89340100	-0.89162800	-0.54924200

4 TEEDA, conformation 2

C	-0.48654000	-0.86434700	-1.12079400
C	0.79768100	-0.03215400	-1.19956500
N	1.68062300	-0.16940600	-0.04037300
N	-1.55847600	-0.29648100	-0.29356300
C	3.03673400	0.28339400	-0.36314500
C	1.13790400	0.40221600	1.20312000
C	-2.49748100	-1.33470200	0.14567200
C	-2.24216000	0.80978300	-0.97014300
H	-0.21051200	-1.83982800	-0.71299300
H	-0.85451000	-1.04004000	-2.15149100
H	1.35732900	-0.40121300	-2.06636600
H	0.55859700	1.02375400	-1.42467200
H	3.06633700	1.36002800	-0.62198700
H	3.34519000	-0.25584300	-1.26640500
H	1.76460600	0.05423900	2.03042200
H	0.14657800	-0.02689200	1.34647400
H	-3.42422400	-0.84495600	0.45668900
H	-2.76695800	-1.99955200	-0.69896800

H	-1.49330500	1.37711000	-1.52971100
H	-2.96348900	0.42758400	-1.72019800
C	-2.94056500	1.76085100	0.00108900
H	-3.41106300	2.58481800	-0.54640700
H	-3.72352500	1.26041300	0.57924900
H	-2.21605100	2.17816000	0.70682000
C	-1.96978800	-2.16029400	1.31880300
H	-1.78813300	-1.51675000	2.18512700
H	-2.69958500	-2.92660200	1.60174700
H	-1.03140800	-2.66844300	1.07701900
C	1.02194200	1.93416100	1.25835700
H	0.58334500	2.23499000	2.21612700
H	1.99425500	2.42988900	1.16863100
H	0.37251700	2.31822400	0.46535500
C	4.05223800	0.00275300	0.74290300
H	3.88832000	0.62634200	1.62688700
H	4.00369900	-1.04718000	1.04987500
H	5.06339800	0.21095000	0.37812400

4 TEEDA, transition state 1-2

C	-0.39171700	-0.95131500	-0.95817300
C	0.91389100	-0.15736000	-1.06556900
N	1.68125400	-0.10314700	0.17567700
N	-1.49763900	-0.25786700	-0.28616300
C	3.11770400	0.13978900	-0.01573300
C	1.09345400	0.68856400	1.26219500
C	-2.46897600	-1.21437100	0.25719600
C	-2.13079100	0.72760100	-1.16759300
H	-0.16289700	-1.86368800	-0.40224200
H	-0.70047100	-1.26223700	-1.97668400
H	1.53352300	-0.68292200	-1.79959000
H	0.71800200	0.84363400	-1.49309600
H	3.42513500	1.05431300	0.51017800
H	3.32966200	0.32468900	-1.07701800
H	1.73760800	0.55399100	2.13951200
H	0.11993000	0.26047100	1.50484000
H	-3.40626200	-0.68225100	0.43961500
H	-2.69968600	-2.00156000	-0.48788300
H	-1.34032100	1.21845300	-1.74249100
H	-2.78709600	0.22875900	-1.90932700
C	-2.91148600	1.80008000	-0.40864900

H	-3.32318800	2.53449700	-1.10939200
H	-3.74922200	1.38170200	0.15756400
H	-2.25510700	2.31933400	0.29590700
C	-2.01039500	-1.84899500	1.56982700
H	-1.87543200	-1.08013700	2.33682000
H	-2.75724100	-2.56722900	1.92523100
H	-1.06124800	-2.38225200	1.46057000
C	0.91350800	2.18900400	0.98020000
H	0.51999900	2.69382200	1.86963400
H	1.85818100	2.67418900	0.71087800
H	0.20240100	2.35606700	0.16601700
C	3.96288700	-1.03688800	0.47802200
H	3.77247600	-1.22485500	1.53987100
H	3.70777200	-1.94874800	-0.07178700
H	5.03387000	-0.83803000	0.34799800

5 DiPyr, conformation 1

C	0.14712100	1.19634000	4.58608900
C	2.06116800	2.03665400	3.59975200
H	-0.77475700	0.62563200	4.45028100
H	2.67419900	2.08153400	2.69815800
C	0.34141500	2.78255900	1.15065700
H	0.34483600	1.80299100	0.63650700
H	1.37119500	3.14986800	1.14795800
C	0.07702500	4.16432600	-0.84165200
C	-1.83701100	3.32399000	0.14467200
C	-1.05615400	4.97847300	-1.47849500
H	0.31514800	3.28348400	-1.46942200
H	0.99891400	4.73501600	-0.70584900
C	-2.34679800	4.36599500	-0.86843200
H	-2.45005000	3.27909800	1.04625900
H	-1.83393400	2.31415800	-0.30946500
H	-0.96626900	6.02970400	-1.19955200
H	-1.03591200	4.92074800	-2.56806200
H	-2.93847200	5.13464800	-0.36886400
H	-2.98372600	3.90193700	-1.62338400
N	-0.47374600	3.76008400	0.45009000
N	0.69789500	1.60057800	3.29434600
C	-0.11726000	2.57810800	2.59378000
H	-1.14704200	2.21080600	2.59647900
H	-0.12067600	3.55767600	3.10793200

C	2.57094900	0.99464200	4.61284900
H	3.16257300	0.22596200	4.11326300
H	3.20792100	1.45868100	5.36777600
C	1.28030500	0.38221700	5.22296100
H	1.26008100	0.44001600	6.31252500
H	1.19040500	-0.66903100	4.94409200
H	-0.09102600	2.07718500	5.21384500
H	2.05811100	3.04648600	4.05388700

5 DiPyr, conformation 2

C	-2.95114300	-1.19203800	-0.44688300
C	-2.54008300	1.07259600	-0.23694600
H	-2.75695200	-2.19493700	-0.05885000
H	-2.06070700	1.85854200	0.34938300
C	0.40741700	0.41250000	0.29019200
H	0.24723300	0.31777400	1.37676900
H	0.23869900	1.46100700	0.03345900
C	2.74960100	1.11952700	0.13006500
C	2.31321700	-1.08649100	0.60138000
H	2.34164400	2.09924900	-0.12266500
H	1.54130800	-1.83534500	0.78114500
N	1.76651500	0.06317500	-0.13587800
N	-1.97187700	-0.23992100	0.07217600
C	-0.62500800	-0.45560400	-0.42796400
H	-0.37521500	-1.50905300	-0.27222800
H	-0.55117100	-0.26781800	-1.51527700
C	-4.03793100	0.91866600	0.08590500
H	-4.25892400	1.29585000	1.08563300
H	-4.65299800	1.48039500	-0.61918700
C	-4.29607000	-0.61134700	0.00861300
H	-5.10354300	-0.86845200	-0.67898100
H	-4.56070000	-1.00194100	0.99269100
H	-2.91169700	-1.24521000	-1.55232500
H	-2.39993500	1.31978400	-1.30723900
C	3.15883800	0.97792300	1.61731500
H	4.18810000	1.29695500	1.79252700
H	2.51508000	1.59352800	2.24968600
C	2.93879100	-0.52793400	1.91290400
H	2.26447600	-0.66581700	2.76014400
H	3.87027200	-1.04301100	2.15569600
H	3.08701400	-1.55533100	-0.01416300

H	3.61917400	0.94663300	-0.51334800
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5 DiPyr, transition state 1-2

C	-2.84870300	-1.00928800	-0.65373200
C	-2.34363000	1.12746900	0.06679600
H	-2.68830800	-2.08125200	-0.51574200
H	-1.82406600	1.73848200	0.80668900
C	0.60033800	0.23061200	0.37757100
H	0.49535400	-0.20182000	1.38178600
H	0.43333400	1.30847000	0.48420200
C	2.64645800	1.00528900	-0.90255800
C	2.69305100	-1.17888500	0.15302800
C	3.91137800	0.25261600	-1.34174700
H	2.90413200	1.89874300	-0.30611800
H	2.06863800	1.35569000	-1.76818800
C	4.12606600	-0.76641000	-0.21066300
H	2.37392800	-2.04510200	-0.45316000
H	2.60207600	-1.47770400	1.20628900
H	3.72023400	-0.27311200	-2.28208000
H	4.76602200	0.91443200	-1.49374200
H	4.75198700	-1.61061100	-0.50612300
H	4.59724400	-0.27721600	0.64707300
N	1.92806100	0.01970000	-0.11945100
N	-1.82348700	-0.24003800	0.04773500
C	-0.49240800	-0.37970200	-0.51612800
H	-0.28153500	-1.44723000	-0.63023900
H	-0.42866900	0.07024500	-1.52667100
C	-3.84135800	0.95569300	0.38181900
H	-4.03141100	1.09784100	1.44681400
H	-4.44432900	1.68731100	-0.15876200
C	-4.16168500	-0.50432400	-0.04154800
H	-4.99055600	-0.56604500	-0.74875800
H	-4.42455800	-1.10382900	0.83165700
H	-2.82972200	-0.80303300	-1.74183200
H	-2.21125300	1.61184400	-0.92052500

6 DiPip, conformation 1

C	-0.50655100	-0.41027500	-0.40168000
C	0.50653600	0.40979100	0.40213100
H	-0.37312400	-0.18719800	-1.47469900
H	-0.29034500	-1.47313500	-0.27324100

H	0.37335000	0.18643800	1.47512600
H	0.29006800	1.47263400	0.27398800
C	-2.42259300	1.08303800	-0.44139300
C	-2.76264400	-1.29685600	-0.29355800
C	-3.78990700	1.36965400	0.17835300
H	-2.51413600	1.06788400	-1.54646100
H	-1.72931300	1.88796600	-0.19132000
C	-4.14422400	-1.11044700	0.33292700
H	-2.87036400	-1.40153800	-1.39225900
H	-2.30733400	-2.22019900	0.07396800
H	-4.17933100	2.31322700	-0.21611100
H	-3.66379600	1.49202900	1.25928800
H	-4.78966900	-1.94842900	0.05221700
H	-4.03623800	-1.12827900	1.42261400
C	2.76247800	1.29670500	0.29440500
C	2.42275900	-1.08333500	0.44066600
C	4.14403900	1.11091400	-0.33229700
H	2.87025600	1.40066500	1.39316900
H	2.30701000	2.22023100	-0.07246700
C	3.79008200	-1.36933700	-0.17935100
H	2.51435500	-1.06893200	1.54574000
H	1.72958500	-1.88819000	0.19006400
H	4.78938300	1.94880000	-0.05107100
H	4.03598100	1.12945700	-1.42196500
H	4.17966100	-2.31311900	0.21446000
H	3.66392200	-1.49101100	-1.26036000
N	-1.87714300	-0.18394900	0.04615400
N	1.87710400	0.18390600	-0.04598600
C	4.76368600	-0.22114000	0.09972200
H	5.71648200	-0.38825100	-0.41101400
H	4.98108000	-0.18621000	1.17468400
C	-4.76365400	0.22140700	-0.10001800
H	-5.71646000	0.38899000	0.41054300
H	-4.98098200	0.18579200	-1.17497100

6 DiPip, conformation 2

C	-0.69808800	0.32414400	-0.20178100
C	0.49609500	-0.40564600	-0.82476300
H	-0.68914400	0.13302200	0.88190000
H	-0.57981600	1.40263500	-0.32752100
H	0.58259300	-0.10931600	-1.88542900

H	0.28643800	-1.47826900	-0.81801400
C	-2.52241600	-1.31211700	-0.34973100
C	-2.95562200	0.98843100	-0.92765400
H	-1.73755200	-2.06961300	-0.28941100
H	-2.48332700	1.89802700	-1.30765600
C	2.74328300	-1.20418300	-0.41627600
C	2.27235100	1.15382800	-0.26367600
C	3.97465300	-1.06789000	0.47829800
H	3.05261900	-1.12657600	-1.47836500
H	2.29240800	-2.19150000	-0.28548800
C	3.48742100	1.38865500	0.63357900
H	2.55586400	1.32555400	-1.32213300
H	1.49337300	1.87857600	-0.02100500
H	4.71438300	-1.82526200	0.20120100
H	3.67559500	-1.26275500	1.51369500
H	3.87581800	2.39779200	0.46506100
H	3.16468300	1.33109100	1.67854800
N	-1.94337400	-0.06619800	-0.86159800
N	1.73682100	-0.19604300	-0.08656400
C	-3.22736000	-1.15680600	1.00858500
H	-3.68419500	-2.10894900	1.29747300
H	-2.48858000	-0.91551400	1.78096800
C	-3.66746500	1.25399600	0.40828200
H	-4.43758500	2.02096400	0.27487000
H	-2.94715000	1.64893800	1.13450200
H	-3.70247600	0.68359500	-1.67215000
H	-3.24762400	-1.67031400	-1.09088300
C	4.57038300	0.33870300	0.37158800
H	5.40433500	0.46016600	1.06902400
H	4.97626100	0.48295700	-0.63760500
C	-4.28283300	-0.04507300	0.94466300
H	-4.73412700	0.11592600	1.92817800
H	-5.09347300	-0.35852800	0.27363300

6 DiPip, transition state 1-2

C	0.51320600	-0.53745100	0.37207900
C	-0.47640000	0.34959300	-0.38710900
H	0.32846300	-0.43547300	1.45556000
H	0.33553500	-1.58495400	0.11878300
H	-0.35566800	0.16948400	-1.47026000
H	-0.21493000	1.39647900	-0.21519500

C	2.40547800	0.95304100	0.70775400
C	2.79824200	-1.33545600	0.28647100
C	3.64000100	1.49727700	-0.00912600
H	2.64321000	0.69548500	1.75872300
H	1.63646300	1.72641500	0.74095600
C	4.22491300	-1.08060100	-0.24606600
H	2.83828300	-1.52499300	1.37738900
H	2.39264000	-2.23798100	-0.17626100
H	4.17096900	2.17610900	0.66451200
H	3.29724800	2.09971500	-0.85394900
H	4.93254100	-1.50109600	0.47275900
H	4.35952200	-1.65022600	-1.16815100
C	-2.70533500	1.28903700	-0.33141000
C	-2.42439900	-1.10292500	-0.40338600
C	-4.10256100	1.15713600	0.27339300
H	-2.78999400	1.36470000	-1.43453500
H	-2.23196200	2.21060600	0.01759500
C	-3.81142900	-1.33364200	0.19579900
H	-2.49202300	-1.12234800	-1.51025600
H	-1.75967300	-1.91730800	-0.11066600
H	-4.71961000	2.00380700	-0.04277300
H	-4.01489500	1.20254700	1.36410800
H	-4.21780600	-2.27827900	-0.17846100
H	-3.71008900	-1.42697000	1.28224300
N	1.89337600	-0.22489600	0.01164100
N	-1.85429900	0.16433800	0.05509600
C	4.59887400	0.39962900	-0.54272800
H	5.60657900	0.58494800	-0.16407300
H	4.66675200	0.51623700	-1.62534600
C	-4.74877200	-0.16947200	-0.13528200
H	-5.71577900	-0.29786300	0.35971600
H	-4.94322700	-0.15867700	-1.21514100

7 DiAze, conformation 1

C	-3.21577000	1.24290500	0.14347800
C	-4.45233700	0.55858900	0.73786700
C	-4.27548800	-0.91774100	1.12592400
C	-2.51753600	0.46221100	-0.97522600
C	-4.08627300	-1.83677400	-0.09222700
C	-2.64033400	-1.96621700	-0.59401400
H	-3.50647700	2.23088000	-0.23363200

H	-4.77588300	1.12746800	1.61616200
H	-5.17229900	-1.23452800	1.66801600
H	-4.43984000	-2.84591600	0.14062800
H	-1.76110700	1.10636900	-1.43017500
H	-2.47376600	1.40564000	0.93193100
H	-5.27665700	0.62061800	0.01557900
H	-3.43184000	-1.02969000	1.81426800
H	-3.22664000	0.21771900	-1.78203000
H	-4.73154800	-1.47645700	-0.90046300
H	-2.12720900	-2.73346200	-0.00504500
H	-2.66211300	-2.33204800	-1.63897000
C	-0.48246800	-0.90455500	-0.91262000
H	-0.36796700	-0.75299200	-2.00053500
H	-0.18629700	-1.93521400	-0.70527300
N	-1.85868600	-0.74235100	-0.46228600
C	0.46206200	0.05364400	-0.17954000
H	0.42605100	-0.19511400	0.89741000
H	0.07688100	1.07082700	-0.28145700
C	2.59298100	1.22455400	-0.39677500
C	2.45888000	-1.26866200	-0.48660300
C	3.27404700	1.28435400	0.98687300
H	3.36202100	1.36440600	-1.16508100
H	1.90993700	2.06994700	-0.50601500
C	3.98744300	-1.29650500	-0.57840500
H	2.05623400	-1.97550800	-1.21874900
H	2.17673500	-1.66549700	0.50756700
C	4.67506300	0.66392100	0.98241600
H	2.63891500	0.79842200	1.73663900
H	3.35914300	2.33338600	1.29004900
C	4.71143800	-0.84071200	0.69851500
H	4.27274600	-2.33493200	-0.77417100
H	4.32600100	-0.72309600	-1.44774200
H	5.16642500	0.85202800	1.94301900
H	5.27489300	1.18472400	0.22464300
H	5.75811400	-1.15911500	0.64675200
H	4.27080500	-1.37789900	1.54785600
N	1.81540500	0.02969600	-0.71937800

7 DiAze, conformation 2

C	-1.62616000	1.68490300	2.77531800
C	-0.32452400	1.76889500	1.96927100

C	-0.48993900	1.94868900	0.45201400
C	-2.67094100	0.71291100	2.21718800
C	-1.08714200	0.70957900	-0.23546200
C	-2.62198600	0.64317900	-0.24184500
H	-1.38463200	1.40180500	3.80698200
H	0.27853300	2.59194200	2.36753300
H	0.49912900	2.14356200	0.02506900
H	-0.75613400	0.66263100	-1.27749200
H	-3.47746600	0.61069800	2.94748500
H	-2.09636600	2.67280400	2.81514400
H	0.25980900	0.85510600	2.13836300
H	-1.10644100	2.82797900	0.24024700
H	-2.24283600	-0.29543100	2.10108100
H	-0.67650600	-0.18442000	0.24582800
H	-2.99903500	1.22417100	-1.08993800
H	-2.92836800	-0.40640600	-0.41704400
C	-4.69559500	1.16275200	0.90851600
H	-5.11197600	0.19688700	1.24283400
H	-4.99627900	1.28386100	-0.13510000
N	-3.23953300	1.19814600	0.95648700
C	-5.31783400	2.28265400	1.74777100
H	-4.91864700	3.25084900	1.39969400
H	-4.98125100	2.17128100	2.78173100
C	-7.31937000	2.75029400	3.01006700
C	-7.37747400	2.76041700	0.51918700
C	-8.83636600	2.96573700	3.03256600
H	-7.04818700	2.02715700	3.78628400
H	-6.83964600	3.70448700	3.29979400
C	-7.70867500	4.26628900	0.47217500
H	-8.29601700	2.20146200	0.30442300
H	-6.69147300	2.51769400	-0.29365400
C	-9.27876700	4.34629400	2.52512400
H	-9.16550300	2.86705200	4.07153900
H	-9.33397900	2.16262300	2.47870500
C	-9.10453800	4.58522200	1.02199900
H	-6.94084500	4.83872100	1.00547400
H	-7.66581200	4.59580800	-0.57117600
H	-8.71038600	5.10585600	3.07645700
H	-10.33080800	4.50524600	2.78497000
H	-9.35855500	5.62743800	0.80118700
H	-9.83098000	3.97084800	0.47450300

N	-6.77683500	2.23748700	1.74966400
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7 DiAze, transition state 1-2

C	-3.27154600	1.70617000	0.29840400
C	-4.49507500	0.98777900	0.87940800
C	-4.29487200	-0.49589600	1.22617500
C	-2.56792300	0.96599900	-0.84419100
C	-4.09798900	-1.37877800	-0.01734300
C	-2.65261600	-1.47317800	-0.52848600
H	-3.57856100	2.69954200	-0.05058000
H	-4.82261700	1.52762000	1.77440000
H	-5.18433500	-0.84044700	1.76342200
H	-4.43588000	-2.39889500	0.18954200
H	-1.82352100	1.63343900	-1.28527500
H	-2.52790100	1.85865500	1.08731900
H	-5.32377200	1.05736900	0.16282700
H	-3.44635000	-0.61398500	1.90749200
H	-3.27780200	0.73293100	-1.65376900
H	-4.75209700	-1.00616100	-0.81281600
H	-2.12560600	-2.24850500	0.03727700
H	-2.67361300	-1.81109000	-1.58280100
C	-0.51260200	-0.37095500	-0.82753300
H	-0.40613200	-0.20113700	-1.91331600
H	-0.19337800	-1.39981200	-0.64246700
N	-1.88862100	-0.24182500	-0.36704300
C	0.43068300	0.58392100	-0.08802500
H	0.33919000	0.39094600	0.99567000
H	0.09232800	1.60987300	-0.25024600
C	2.55148700	1.72397800	-0.46923000
C	2.45734000	-0.77364100	-0.14152000
H	1.88604000	2.50306100	-0.84868300
H	2.78984800	2.00864900	0.57358200
C	3.83956300	1.75375500	-1.30319400
C	3.78910000	-0.67507400	0.61405600
H	1.75776000	-1.31157300	0.50784400
H	2.61772900	-1.42133100	-1.01486800
H	4.04062000	2.79502700	-1.57593700
H	3.65411300	1.21388900	-2.23834100
C	5.07691300	1.19824100	-0.59478200
H	3.97085900	-1.66865900	1.03721300
H	3.69736600	0.00509200	1.46816200

C	4.99823600	-0.28897800	-0.24723000
H	5.96003100	1.37439700	-1.21833500
H	5.23459900	1.76986800	0.32892800
H	5.91694800	-0.57489300	0.27577300
H	4.97243900	-0.88156900	-1.17079200
N	1.80220900	0.47671100	-0.56815800

8 MeDiPip, conformation 1

C	-0.51422400	-0.41679400	-0.38702300
C	0.51449500	0.37118800	0.42875300
H	-0.39282200	-0.16098000	-1.45402000
H	-0.30678300	-1.48490800	-0.29425100
H	0.41821100	0.08829500	1.49176300
H	0.27961700	1.43595300	0.36576200
C	-2.42480000	1.08346200	-0.37158400
C	-2.77896100	-1.28843900	-0.25229300
C	-3.76790300	1.39567800	0.29459400
H	-2.56032100	1.07681500	-1.47329000
H	-1.71481900	1.88155700	-0.14477700
C	-4.13537700	-1.12467400	0.44609700
H	-2.93714900	-1.35161500	-1.34720200
H	-2.31262300	-2.22617200	0.06230900
H	-3.58235800	1.48590800	1.37043500
C	2.75850900	1.28131400	0.33143400
C	2.44125400	-1.10158400	0.30019700
C	4.12859600	1.17430200	-0.34240800
H	2.90025600	1.29984600	1.43193500
H	2.28612900	2.22760900	0.05287600
C	3.79409200	-1.34143700	-0.37463700
H	2.56734200	-1.17405900	1.40043200
H	1.74785200	-1.89255200	0.00742800
H	3.95700200	1.23639200	-1.42388300
H	3.61752800	-1.33162800	-1.45701400
N	-1.87596000	-0.19083500	0.08627400
N	1.87382300	0.19207200	-0.07176600
C	4.74977800	-0.19270300	-0.03658600
H	5.69239400	-0.31069300	-0.58215700
H	4.99745900	-0.23965500	1.03345700
C	-4.74157600	0.23432700	0.05861900
H	-5.67348100	0.40491800	0.60812100
H	-5.00309100	0.21521000	-1.00749000

C	-4.33719300	2.72106500	-0.21231100
H	-5.28584100	2.95355800	0.27910600
H	-3.64928800	3.55017500	-0.02172800
H	-4.52225000	2.68033400	-1.29070000
C	5.04341900	2.32370800	0.08103400
H	6.01326500	2.25727700	-0.41946700
H	4.60503200	3.29514000	-0.16566400
H	5.22415000	2.30211200	1.16067600
C	4.37337600	-2.70016100	0.02008300
H	3.69727700	-3.51660000	-0.25029800
H	5.32975700	-2.87847000	-0.47892800
H	4.54680100	-2.75247400	1.09986300
H	-4.79576300	-1.91179200	0.06388900
C	-4.00487400	-1.30338600	1.96315800
H	-4.96097100	-1.12622400	2.46387100
H	-3.68255800	-2.32028700	2.20560400
H	-3.26397300	-0.61695600	2.37499200

8 MeDiPip, conformation 2

C	-0.63990400	0.51721700	-0.09811700
C	0.48368500	-0.38480700	-0.61307100
H	-0.71574300	0.37034300	0.98913600
H	-0.34569500	1.56017500	-0.24386000
H	0.51701600	-0.32795500	-1.71495000
H	0.26307800	-1.42281400	-0.35486400
C	-2.50948900	-0.98718600	-0.81378400
C	-2.87973700	1.37678100	-0.57668400
H	-1.74434500	-1.74872400	-0.97528000
H	-2.37821700	2.34919700	-0.58928500
C	2.68209200	-1.17593700	0.05887900
C	2.39838600	1.10812000	-0.63573900
C	3.93478100	-0.84126300	0.87263200
H	2.98971300	-1.50095300	-0.95658600
H	2.15954900	-2.01796900	0.52149400
C	3.63361900	1.57176000	0.13990000
H	2.69480500	0.86712100	-1.67748400
H	1.67678100	1.92583100	-0.69351400
H	3.59860500	-0.60207700	1.88883600
H	3.29251200	1.86332900	1.14063100

N	-1.88885600	0.33743600	-0.83204500
N	1.76374400	-0.04299000	0.00054300
C	-3.34849700	-1.33246700	0.43772200
H	-3.93272800	-2.22461200	0.17784900
C	-3.66613700	1.19338300	0.73462800
H	-3.59691400	1.37647000	-1.41021900
H	-3.17779600	-1.03174800	-1.68350800
C	4.61361600	0.40337300	0.29050100
H	5.46256100	0.69874000	0.91671100
H	5.02378100	0.15470100	-0.69867200
C	-4.33953100	-0.18733400	0.71856500
H	-4.86501100	-0.36501600	1.66361800
H	-5.10618000	-0.18041700	-0.06781300
C	4.28611400	2.77985200	-0.53256800
H	3.58837500	3.61878200	-0.61063000
H	5.15740900	3.12052000	0.03337700
H	4.62339300	2.52967800	-1.54370100
C	4.88861900	-2.03445200	0.93408800
H	5.77088400	-1.80017700	1.53593400
H	4.40476600	-2.91046600	1.37595500
H	5.23329700	-2.31153500	-0.06749600
C	-2.50883000	-1.69018000	1.67122700
H	-3.14744300	-2.09024600	2.46438400
H	-1.76014300	-2.45107500	1.43179600
H	-1.98171500	-0.82746800	2.08089100
C	-4.68584600	2.31455200	0.92970300
H	-5.24793200	2.18294500	1.85869800
H	-4.19950400	3.29389400	0.96752500
H	-5.40680700	2.33161400	0.10521900
H	-2.95208500	1.23055500	1.56603900

8 MeDiPip, transition state 1-2

C	-0.49510700	-0.52003600	-0.33949000
C	0.51951100	0.33544200	0.42283500
H	-0.36463900	-0.35045600	-1.42223000
H	-0.29105000	-1.57745000	-0.15832800
H	0.44110700	0.10396800	1.49988100
H	0.24932300	1.38805600	0.31037900
C	-2.41883700	0.95861100	-0.48618100
C	-2.77124200	-1.34896100	-0.19410800
C	-3.63882100	1.44548400	0.30074000

H	-2.69597700	0.76827500	-1.54291700
H	-1.66629900	1.74915600	-0.49803300
C	-4.13594100	-1.18525500	0.50983500
H	-2.92103000	-1.42949300	-1.28866100
H	-2.31110000	-2.28498000	0.13231600
H	-3.24436300	1.99517300	1.16092400
C	2.73954200	1.29213500	0.29974000
C	2.47667700	-1.09805200	0.31340900
C	4.11141300	1.20398400	-0.37296400
H	2.88116700	1.33496100	1.39957400
H	2.24509300	2.22182900	0.00391100
C	3.83550400	-1.31849500	-0.35610300
H	2.60276700	-1.14893400	1.41490600
H	1.80250400	-1.90972600	0.03288400
H	3.93829700	1.24040000	-1.45537200
H	3.65965400	-1.33344800	-1.43854700
N	-1.86016300	-0.25224400	0.10545000
N	1.87948600	0.17544300	-0.08137200
C	-4.50550400	0.28583000	0.86976100
H	-5.54883600	0.45236600	0.58729700
H	-4.48328500	0.36884400	1.95873000
C	4.76412900	-0.14175800	-0.04008900
H	5.70964300	-0.24861000	-0.58293000
H	5.01193100	-0.16188600	1.03075800
C	4.99915400	2.38273200	0.02675500
H	5.97015200	2.32896500	-0.47303600
H	4.53809200	3.33849500	-0.23906000
H	5.18062800	2.38703900	1.10647600
C	4.44583600	-2.65572500	0.06446100
H	3.78880200	-3.49256400	-0.19007800
H	5.40617700	-2.82144700	-0.43126100
H	4.62018800	-2.68334400	1.14500300
C	-4.46377100	2.42087300	-0.54305300
H	-5.28014900	2.85479900	0.04044300
H	-3.84824200	3.24401500	-0.91982100
H	-4.90280600	1.90982900	-1.40619100
C	-4.18626900	-2.04924100	1.77610900
H	-5.14159600	-1.93789200	2.29706600
H	-4.05257300	-3.10954300	1.54164000
H	-3.38853500	-1.74735200	2.46202700
H	-4.89359200	-1.56516600	-0.18238500

9 DiMph, conformation 1

C	-0.51237800	-0.42901400	-0.37313800
C	0.51227900	0.42175400	0.38017100
H	-0.40387200	-0.24375900	-1.45604100
H	-0.29324900	-1.48680400	-0.20969100
H	0.40390900	0.23633700	1.46306200
H	0.29298900	1.47953800	0.21689900
C	-2.42920100	1.07360300	-0.38425200
C	-2.77712100	-1.28747000	-0.25098500
C	-3.82172100	1.28299100	0.19710800
H	-2.49047500	1.08782700	-1.48868300
H	-1.78640900	1.90054300	-0.07442400
C	-4.15935700	-1.02399000	0.33204300
H	-2.86673100	-1.40994100	-1.34661900
H	-2.37897100	-2.21939300	0.16099800
H	-4.27717800	2.18727900	-0.20938300
H	-3.74751100	1.38033900	1.29039600
H	-4.86289600	-1.80042700	0.02773400
H	-4.09343900	-1.01081700	1.43010200
C	2.77693600	1.28038900	0.25835300
C	2.42917600	-1.08077000	0.39056600
C	4.15920200	1.01726700	-0.32476000
H	2.86651500	1.40238900	1.35404200
H	2.37872600	2.21246500	-0.15322800
C	3.82173000	-1.28979400	-0.19084600
H	2.49041300	-1.09550100	1.49499400
H	1.78646000	-1.90761500	0.08033100
H	4.86267500	1.79362300	-0.02009600
H	4.09331300	1.00456900	-1.42282700
H	4.27724000	-2.19422900	0.21525700
H	3.74755800	-1.38666600	-1.28417900
N	-1.87334800	-0.19174100	0.09550500
N	1.87324000	0.18475200	-0.08862800
O	4.68923000	-0.21559800	0.14325100
O	-4.68930500	0.20870900	-0.13649300

9 DiMph, conformation 2

C	-0.42284000	-0.42164400	-0.40456400
C	0.58152600	0.37579900	0.43237600
H	-0.19706800	-0.25126800	-1.46788700
H	-0.28841500	-1.49058900	-0.22510500

H	0.47091200	0.08930800	1.49309700
H	0.32440500	1.43647200	0.36715700
C	-2.30949300	1.12778100	-0.68840800
C	-2.76619000	-1.16186000	-0.14258400
H	-1.54291700	1.90687000	-0.68466800
H	-2.34085000	-2.07375600	0.28527300
C	2.83692500	1.24722800	0.52370200
C	2.50452600	-1.10112100	0.21727400
C	4.23852000	1.09760300	-0.05268800
H	2.89191300	1.17083000	1.62575300
H	2.44200800	2.23668100	0.27472200
C	3.91728700	-1.19667600	-0.34521600
H	2.52855500	-1.31954000	1.30164100
H	1.88023900	-1.85776500	-0.26337200
H	4.92542300	1.80900100	0.40826800
H	4.20744700	1.28110800	-1.13698700
H	4.36784800	-2.15815800	-0.09423900
H	3.87878400	-1.09509800	-1.44005800
N	-1.79196800	-0.07406800	-0.02284000
N	1.95279500	0.22889900	-0.04093500
O	4.76423700	-0.19768400	0.20453300
C	-2.77870600	0.85048200	-2.11802900
H	-3.26444500	1.72847200	-2.54829500
H	-1.92566200	0.58067900	-2.75928200
C	-3.21818800	-1.39661200	-1.58390500
H	-4.01968500	-2.13660000	-1.63257900
H	-2.37714200	-1.75571400	-2.19799000
O	-3.74538000	-0.19613400	-2.14147000
H	-3.64520100	-0.89338100	0.45448600
H	-3.15921200	1.50010700	-0.10593000

9 DiMph, transition state 1-2

C	-0.51660300	0.54742500	0.33922600
C	0.48003700	-0.36658100	-0.37524500
H	-0.34741600	0.48511500	1.42838700
H	-0.33739200	1.58510000	0.04834800
H	0.38509600	-0.21535700	-1.46483300
H	0.21229100	-1.40793400	-0.17909000
C	-2.41948700	-0.93456600	0.68370100
C	-2.80485500	1.32653000	0.24040300
C	-3.68260200	-1.41430100	-0.01914000

H	-2.62368800	-0.67564500	1.74083700
H	-1.69418800	-1.74985500	0.68585100
C	-4.24463000	0.99062200	-0.21516500
H	-2.80317000	1.56808800	1.32110600
H	-2.45890300	2.21570100	-0.29152100
H	-4.26702000	-2.04929400	0.65926100
H	-3.39559800	-2.01666400	-0.88719900
H	-4.94873100	1.34081900	0.55078400
H	-4.46852600	1.53152400	-1.13783800
C	2.71872100	-1.28092300	-0.30624600
C	2.42964000	1.09264000	-0.34729000
C	4.11565100	-1.07467100	0.26391300
H	2.78880100	-1.36554800	-1.40679200
H	2.30162800	-2.21681800	0.07727400
C	3.83668200	1.24299900	0.21755200
H	2.47207800	1.15027200	-1.45125000
H	1.81504500	1.92259900	0.00832300
H	4.79368800	-1.85759200	-0.07910000
H	4.06717000	-1.09914100	1.36270400
H	4.30931000	2.14990300	-0.16259500
H	3.78220700	1.30141900	1.31482700
N	-1.89206100	0.22378700	-0.02646600
N	1.84800400	-0.17593400	0.09251800
O	4.67035000	0.16004500	-0.16932800
O	-4.51405100	-0.37338200	-0.51693500

10 MeDiPz, conformation 1

C	0.51956500	-0.27151700	0.56269000
C	-0.51955700	-0.27144100	-0.56272900
H	0.37184300	0.59116700	1.23905500
H	0.35197600	-1.17250000	1.16085700
H	-0.35196000	-1.17233600	-1.16102700
H	-0.37184800	0.59134200	-1.23896900
C	2.33193100	0.99777700	-0.45418600
C	2.83088100	-0.80169000	1.05673200
C	3.73220400	0.89138900	-1.05108600
H	2.34193700	1.75276200	0.35656000
H	1.63626500	1.34033700	-1.22455700
C	4.23229800	-0.91620500	0.46390000
H	2.86857400	-0.13397300	1.93965300
H	2.49220200	-1.78775200	1.39147200

H	4.06533000	1.88119400	-1.38006500
H	3.68464800	0.22994700	-1.93553100
H	4.93196400	-1.24668700	1.23863400
H	4.21117800	-1.68101900	-0.33400400
C	-2.33195300	0.99769900	0.45429100
C	-2.83087500	-0.80158500	-1.05682400
C	-3.73221400	0.89121300	1.05119700
H	-2.34198600	1.75276300	-0.35638000
H	-1.63629300	1.34020700	1.22469000
C	-4.23228200	-0.91620800	-0.46399800
H	-2.86858500	-0.13374500	-1.93965100
H	-2.49219000	-1.78759600	-1.39170700
H	-4.06534200	1.88097600	1.38030200
H	-3.68464400	0.22966500	1.93556100
H	-4.93193500	-1.24662000	-1.23877300
H	-4.21114900	-1.68111200	0.33381700
N	1.88874400	-0.30462200	0.05159300
N	-1.88873300	-0.30463300	-0.05163100
N	-4.65329200	0.39522700	0.02902700
H	-5.60150100	0.35487600	0.39008300
N	4.65325700	0.39529800	-0.02895700
H	5.60149400	0.35506800	-0.38994900

10 MeDiPz, conformation 2

C	0.56139400	-0.36016000	0.50651800
C	-0.44285200	-0.31701400	-0.65069600
H	0.35846300	0.45813900	1.22320500
H	0.39889300	-1.29509100	1.05108900
H	-0.31777800	-1.23213300	-1.23732500
H	-0.20613500	0.51665500	-1.33035400
C	2.37934100	1.02469800	-0.32882500
C	2.87117500	-0.89862900	1.02171100
C	3.79442900	0.99492100	-0.89902000
H	2.35900300	1.70013600	0.54913000
H	1.69485600	1.42880700	-1.07974800
C	4.28833400	-0.93786300	0.45690600
H	2.87604700	-0.31456500	1.96269000
H	2.54102700	-1.91602600	1.25590100
H	4.11932300	2.01557400	-1.12653500
H	3.77809500	0.41775500	-1.84175600
H	4.97508700	-1.32690200	1.21584500

H	4.29930200	-1.62699900	-0.40739300
C	-2.27098300	1.08167600	0.21861600
C	-2.81020100	-0.91149500	-1.01186100
H	-1.48872400	1.57876900	0.79981400
H	-2.42775000	-1.88985800	-1.32008700
N	1.94661000	-0.32502700	0.04170600
N	-1.81745000	-0.26756500	-0.14596500
C	-2.65649000	1.94075900	-0.99349800
H	-3.07012200	2.89549100	-0.65096000
H	-1.75301700	2.16552800	-1.59173800
C	-3.18769000	-0.07009000	-2.23707800
H	-3.98503200	-0.56780100	-2.79985800
H	-2.31031000	0.02133000	-2.90598100
H	-3.15105800	0.97781900	0.86496400
H	-3.71714800	-1.07572100	-0.41617200
N	4.69898900	0.41919800	0.09571900
H	5.65604900	0.42577700	-0.24345900
N	-3.67539100	1.23197900	-1.77274100
H	-3.98405000	1.79914600	-2.55613100

10 MeDiPz, transition state 1-2

C	-0.50622600	-0.39586400	-0.52161200
C	0.52936500	-0.32407100	0.60400700
H	-0.35611500	0.41879400	-1.25533300
H	-0.34410000	-1.33446100	-1.06032300
H	0.39977900	-1.21534800	1.22517300
H	0.33817300	0.54620700	1.25973700
C	-2.33224800	0.95204100	0.35501500
C	-2.81499400	-0.91756000	-0.98523100
C	-3.59392000	0.85946000	1.20986300
H	-2.52269500	1.54423200	-0.56502800
H	-1.55906600	1.47610000	0.92155100
C	-4.26522600	-0.97637800	-0.44884200
H	-2.78824100	-0.29110500	-1.90095200
H	-2.49323900	-1.92199000	-1.27479600
H	-4.10517500	1.83371200	1.17762000
H	-3.28986500	0.68648300	2.25190100
H	-4.93139900	-0.63017400	-1.25530800
H	-4.52768000	-2.02420800	-0.25470300
C	2.29353200	1.00909800	-0.41344300
C	2.86095500	-0.77099200	1.09633800

C	3.69387400	0.95151900	-1.01691800
H	2.28155000	1.76375400	0.39754800
H	1.58203800	1.32753400	-1.18003400
C	4.26301700	-0.83679200	0.49763600
H	2.87857300	-0.10193000	1.97872700
H	2.55822100	-1.76804900	1.43270500
H	3.99116500	1.95219400	-1.34741900
H	3.66532900	0.28859500	-1.90109000
H	4.97725300	-1.14152000	1.26959600
H	4.26524600	-1.60278700	-0.29937300
N	-1.87322600	-0.38705400	-0.00443300
N	1.89873000	-0.30773100	0.09407500
N	4.63574900	0.48813400	0.00158800
H	5.58334600	0.48073400	-0.36320300
N	-4.47485000	-0.23370300	0.79688500
H	-5.45042200	-0.00665600	0.92876200

11 iPrDiPz, conformation 1

C	-0.49041100	0.44509500	0.38292600
C	0.49041100	-0.44509500	-0.38292600
H	-0.39358800	0.23598600	1.46289400
H	-0.21519800	1.49244300	0.23807300
H	0.39358800	-0.23598600	-1.46289400
H	0.21519800	-1.49244400	-0.23807300
C	-2.48265900	-0.95130400	0.36236200
C	-2.70809200	1.41209800	0.28869500
C	-3.87976900	-1.10494200	-0.22397800
H	-2.55149100	-0.98023800	1.46617500
H	-1.87696100	-1.80209300	0.04444700
C	-4.10374500	1.26364400	-0.30163800
H	-2.79520800	1.50174300	1.38783500
H	-2.25793800	2.33460100	-0.08833400
H	-4.30656000	-2.02926100	0.16278600
H	-3.79833900	-1.20114600	-1.32309300
H	-4.69997700	2.11497800	0.02373000
H	-4.03130500	1.29963700	-1.40498500
C	2.70809200	-1.41209900	-0.28869400
C	2.48265900	0.95130400	-0.36236200
C	4.10374500	-1.26364400	0.30163800
H	2.79520800	-1.50174400	-1.38783500
H	2.25793800	-2.33460100	0.08833500

C	3.87976900	1.10494200	0.22397800
H	2.55149100	0.98023800	-1.46617600
H	1.87696100	1.80209300	-0.04444700
H	4.69997700	-2.11497800	-0.02373000
H	4.03130500	-1.29963700	1.40498500
H	4.30656000	2.02926100	-0.16278700
H	3.79833900	1.20114600	1.32309300
N	-1.86097400	0.28812600	-0.09066900
N	1.86097400	-0.28812700	0.09066900
N	-4.73658900	0.02222000	0.14724000
N	4.73658900	-0.02222000	-0.14724000
C	6.11950300	0.12430800	0.34433000
H	6.11681800	0.15722800	1.45179600
C	-6.11950300	-0.12430800	-0.34433000
H	-6.11681800	-0.15722800	-1.45179600
C	6.75274900	1.42338100	-0.16812300
H	6.29946000	2.31547100	0.26493800
H	7.81405400	1.44311200	0.08825900
H	6.65872600	1.47978500	-1.25635800
C	6.98894400	-1.06026500	-0.09403300
H	8.03335900	-0.86524500	0.15827900
H	6.70857600	-1.99494400	0.39238900
H	6.91418300	-1.19664300	-1.17664900
C	-6.75274900	-1.42338100	0.16812300
H	-7.81405400	-1.44311200	-0.08825900
H	-6.29946000	-2.31547100	-0.26493800
H	-6.65872700	-1.47978500	1.25635900
C	-6.98894400	1.06026500	0.09403300
H	-6.70857600	1.99494400	-0.39239000
H	-8.03335900	0.86524500	-0.15827900
H	-6.91418300	1.19664400	1.17664800

11 iPrDiPz, conformation 2

C	0.73889500	-0.05390900	0.77988500
C	-0.46569800	-0.98183000	0.95769200
H	0.81918800	0.20837200	-0.28548500
H	0.57024500	0.88081800	1.31939800
H	-0.65572200	-1.11853700	2.03733800
H	-0.20764000	-1.96690800	0.55954200
C	2.61571800	-1.59126600	0.41141000
C	2.93113100	0.26311300	1.86029200

H	1.87597100	-2.24365000	-0.05827300
H	2.42552500	0.99401700	2.49646800
C	-2.66848200	-1.55422000	0.14877600
C	-2.23547100	0.68133900	0.82869700
C	-3.85577600	-1.07746100	-0.67631300
H	-3.03052700	-1.85673500	1.14934200
H	-2.23132200	-2.43551100	-0.32902900
C	-3.42653200	1.16074200	0.00929400
H	-2.56569300	0.49527900	1.86831900
H	-1.48923700	1.47793400	0.85325200
H	-4.59366900	-1.87812200	-0.69980100
H	-3.52041300	-0.89209000	-1.71419300
H	-3.84189500	2.03847500	0.50237200
H	-3.07079100	1.46934500	-0.99191100
N	1.94471900	-0.67309200	1.33069800
N	-1.64791600	-0.51783300	0.24203700
C	3.43877200	-0.88760300	-0.67302900
H	3.94620100	-1.65356100	-1.25834400
H	2.76870800	-0.33899000	-1.36268900
C	3.74782500	0.98344700	0.78367900
H	4.48549600	1.61221400	1.28124900
H	3.09032300	1.65062600	0.19200300
H	3.62622500	-0.30202700	2.49134700
H	3.28838400	-2.22659600	0.99737900
N	-4.45424200	0.12356100	-0.09101400
N	4.43145400	0.01427100	-0.07872600
C	-5.65507000	0.57672600	-0.81766400
H	-5.38013600	0.84162500	-1.85782300
C	5.29038700	0.65785300	-1.09107700
H	4.66567500	1.27781300	-1.76456200
C	6.33114300	1.57184100	-0.43345700
H	7.03944500	1.92578500	-1.18550600
H	5.88804600	2.45224000	0.03279800
H	6.88515700	1.01735600	0.32945200
C	6.01610200	-0.38835200	-1.94550400
H	6.54420200	-1.09545200	-1.29934800
H	5.34148700	-0.94903400	-2.59296600
H	6.74784300	0.10384700	-2.58956300
C	-6.71597400	-0.52899500	-0.87327100
H	-7.64390700	-0.13013400	-1.28848000
H	-6.41837200	-1.37108000	-1.49869600

H	-6.91970900	-0.90074500	0.13499100
C	-6.26446700	1.81867500	-0.15623100
H	-6.43300800	1.62927000	0.90774300
H	-5.63482200	2.70342300	-0.25450700
H	-7.22436600	2.05178300	-0.62184600

11 iPrDiPz, transition state 1-2

C	0.49139300	-0.59410500	0.53968000
C	-0.42109000	0.36346300	-0.22847500
H	0.29030000	-0.49205200	1.62082200
H	0.25174800	-1.62431000	0.26702400
H	-0.27690800	0.20125900	-1.31123000
H	-0.11410500	1.39176700	-0.02210500
C	2.46213600	0.76954600	0.92118500
C	2.73448800	-1.50960600	0.56344500
C	3.83972800	1.13880200	0.37141700
H	2.53112100	0.53687700	2.00220200
H	1.81133100	1.63916400	0.82112500
C	4.15023900	-1.35920900	-0.00001400
H	2.77574700	-1.62488300	1.66466600
H	2.29774900	-2.42472900	0.15743200
H	4.36206000	1.68701100	1.16925800
H	3.69836700	1.84701500	-0.45514800
H	4.81007200	-1.96797100	0.63566400
H	4.16924700	-1.81552500	-0.99780200
C	-2.61153300	1.38678000	-0.25677800
C	-2.44558600	-0.98253300	-0.32234600
C	-4.04324500	1.27577500	0.24911000
H	-2.63064700	1.47980900	-1.35884200
H	-2.15925100	2.29632600	0.14832600
C	-3.87940100	-1.09744700	0.17812900
H	-2.44766300	-1.01133100	-1.42832800
H	-1.88439600	-1.84911100	0.03252900
H	-4.59555700	2.14367100	-0.10837900
H	-4.03598700	1.30777900	1.35494400
H	-4.30716100	-2.00960000	-0.23546400
H	-3.86701200	-1.19645700	1.27997900
N	1.89724000	-0.37206000	0.21435700
N	-1.81858700	0.23982900	0.16868700
N	-4.68125600	0.05287300	-0.24112700
N	4.64157800	0.01227600	-0.09416300

C	6.09176800	0.18218500	-0.02426200
H	6.44263900	0.07470400	1.02427400
C	-6.09511200	-0.05708100	0.16449300
H	-6.16107300	-0.09394600	1.26987800
C	-6.73091700	-1.33639900	-0.39257600
H	-6.32922400	-2.24225700	0.06231400
H	-7.80602300	-1.32811100	-0.20130800
H	-6.57226200	-1.39114100	-1.47338400
C	-6.90342400	1.15249500	-0.31997900
H	-7.96633100	0.98506600	-0.13368300
H	-6.62854400	2.07718700	0.18816800
H	-6.75822100	1.29108300	-1.39515400
C	6.51773000	1.57091100	-0.51947400
H	6.11363800	2.38132300	0.08737100
H	7.60695000	1.65153800	-0.49228000
H	6.18620400	1.71667200	-1.55168800
C	6.82198400	-0.86896800	-0.87096700
H	7.89867000	-0.68820700	-0.83022600
H	6.64739000	-1.88852000	-0.52695400
H	6.49935400	-0.79817800	-1.91381400