

Electronic Supplementary Information

**A new route to the efficient metalation of
unfunctionalized aromatics**

Andrew J. Peel,^a Noriyuki Tezuka,^{b,c} James M. D’Rozario,^a Masanobu Uchiyama^{*b,c} and Andrew
E. H. Wheatley^{*a}

^a*Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge, CB2 1EW (UK);*

Fax: (+) 44 1223 336362; e-mail: aeHW2@cam.ac.uk

^b*Cluster of Pioneering Research (CPR), Advanced Elements Chemistry Laboratory, RIKEN, 2-1*

Hirosawa, Wako-shi, Saitama 351-0198 (Japan)

^c*Graduate School of Pharmaceutical Sciences, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku,*

Tokyo 113-0033 (Japan); e-mail: uchiYama@mol.f.u-tokyo.ac.jp

Additional characterisation of **1**

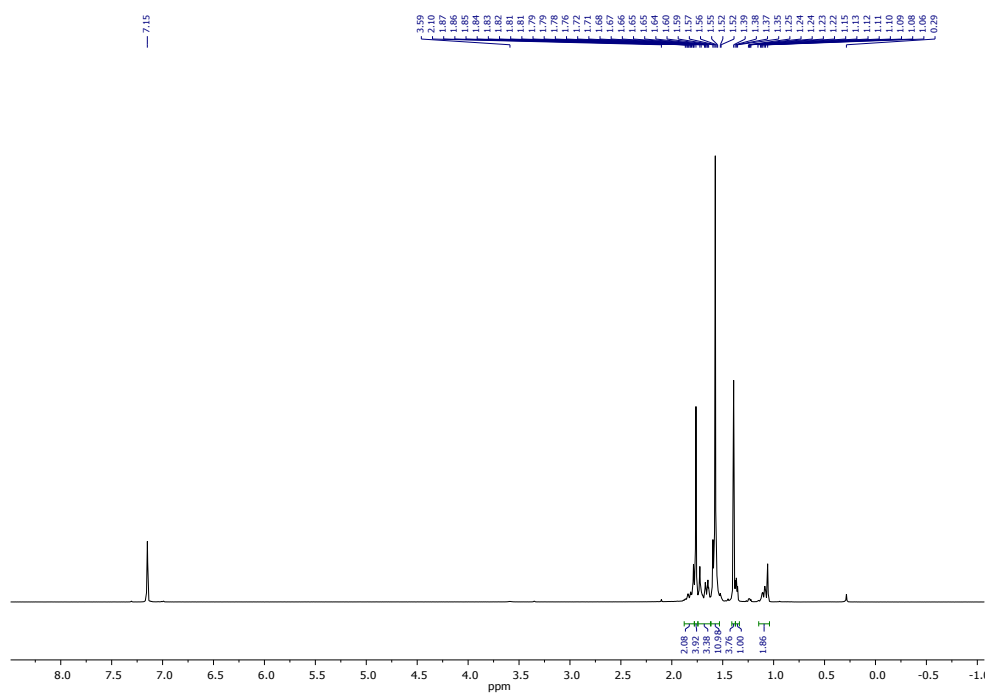


Figure S1a ¹H NMR spectrum of **1** (500 MHz, 298 K, C₆D₆).

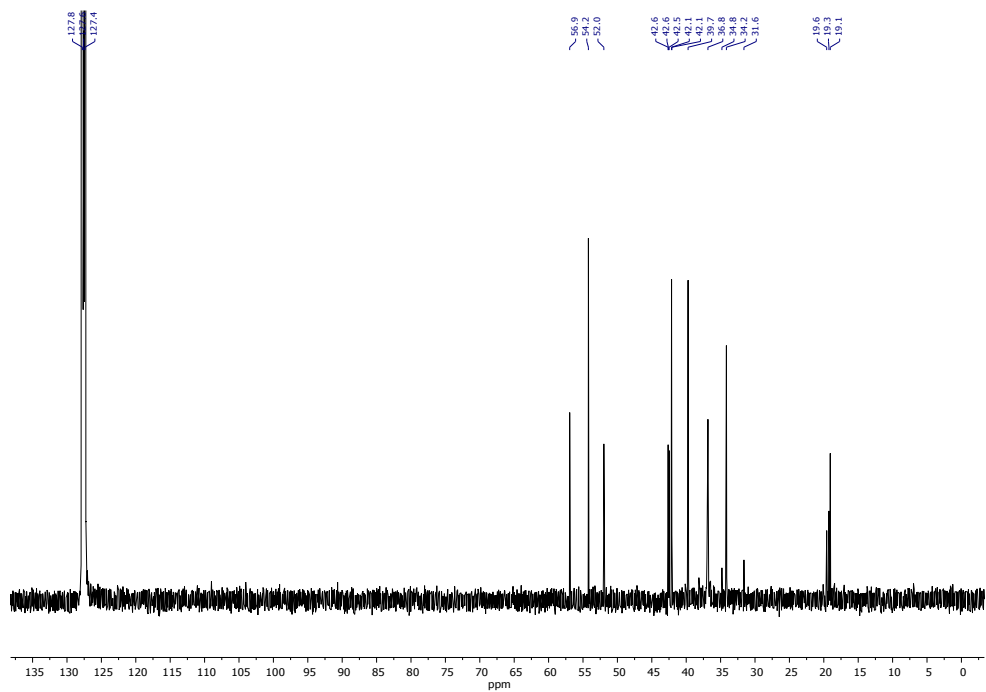


Figure S1b ¹³C NMR spectrum of **1** (125 MHz, 298 K, C₆D₆).

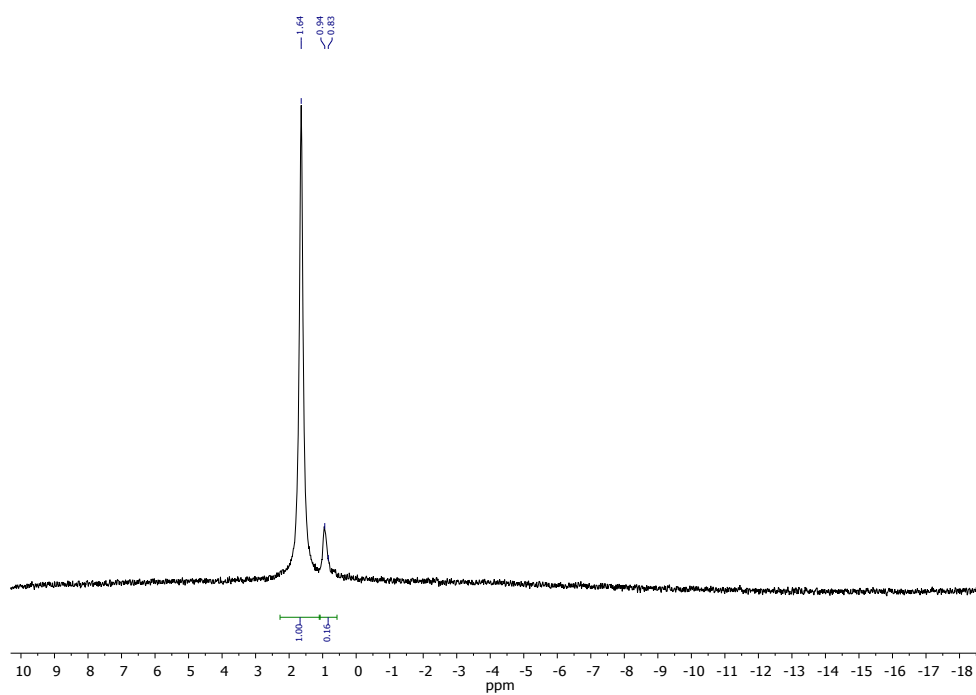


Figure S1c ^7Li NMR spectrum of **1** (194 MHz, 298 K, C_6D_6).

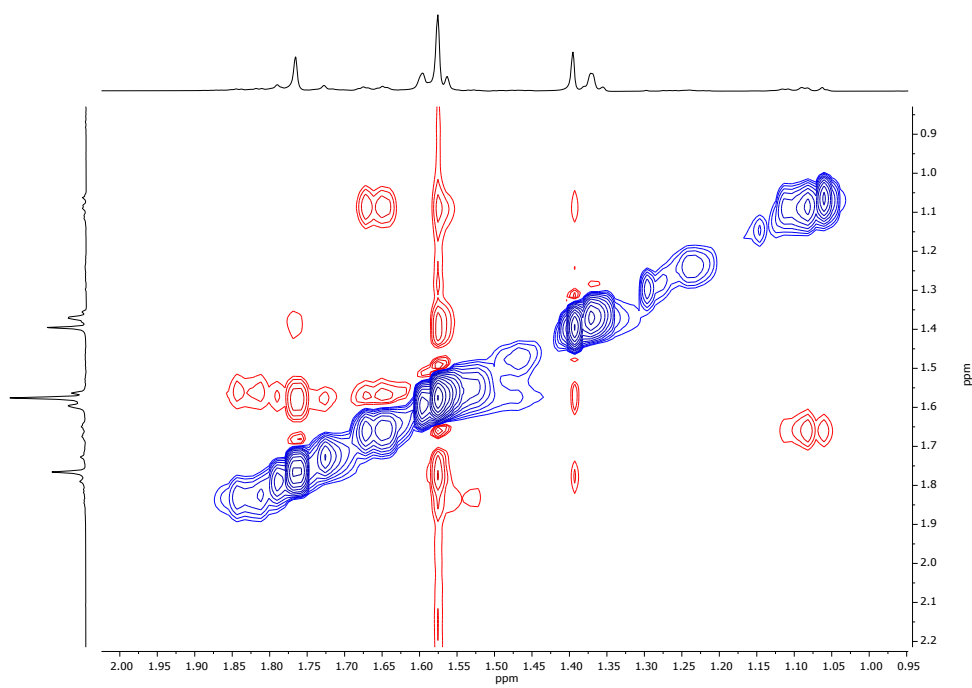


Figure S1d ^1H , ^1H -NOESY spectrum of **1** (500 MHz, 298 K, C_6D_6 , $\tau = 0.6$ s).

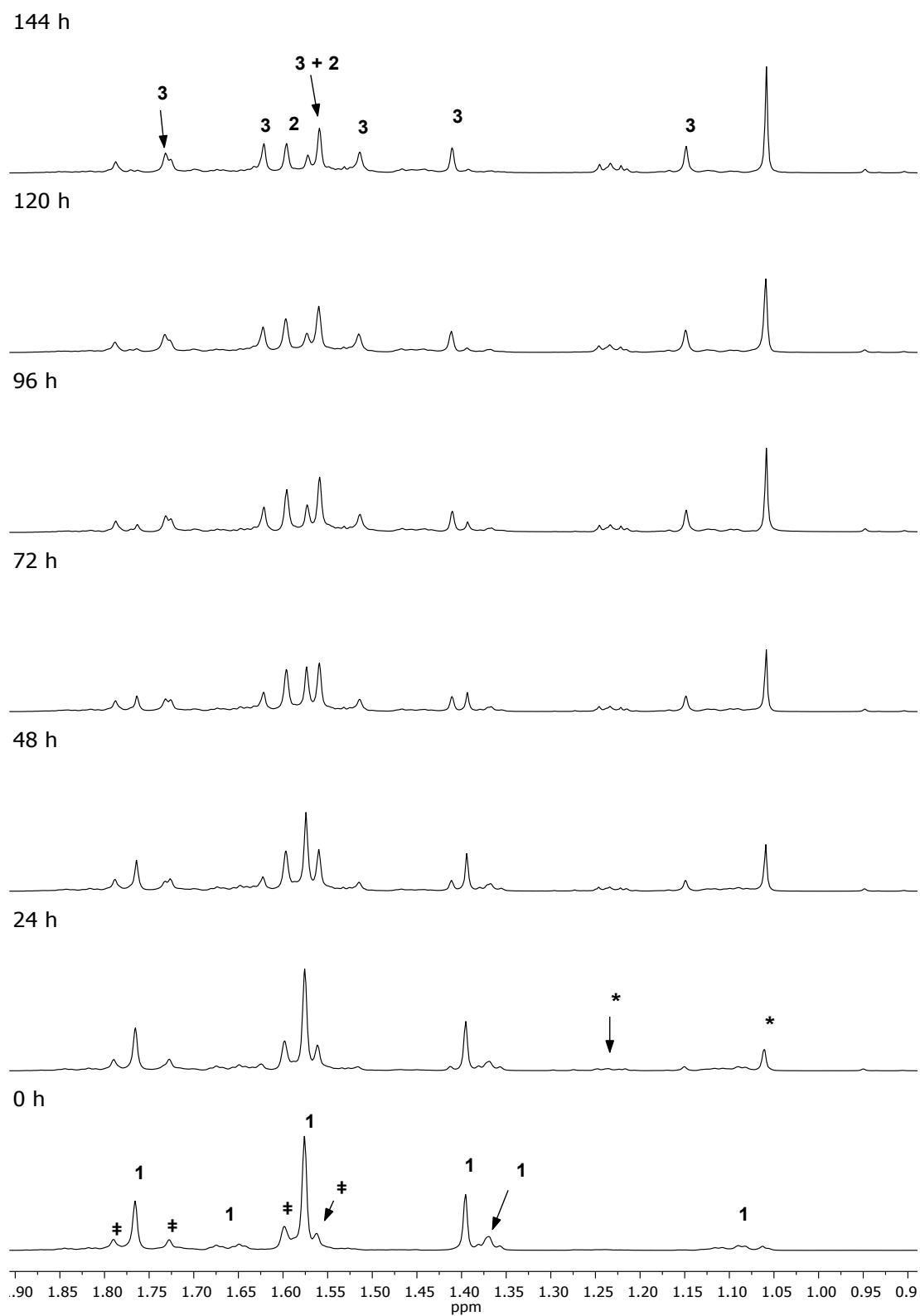


Figure S1e ^1H NMR spectra (500 MHz, 298 K, C_6D_6) of **1** heated to 50°C for the time specified. * = TMPH, ‡ = Cu-rich TMP-aggregate.

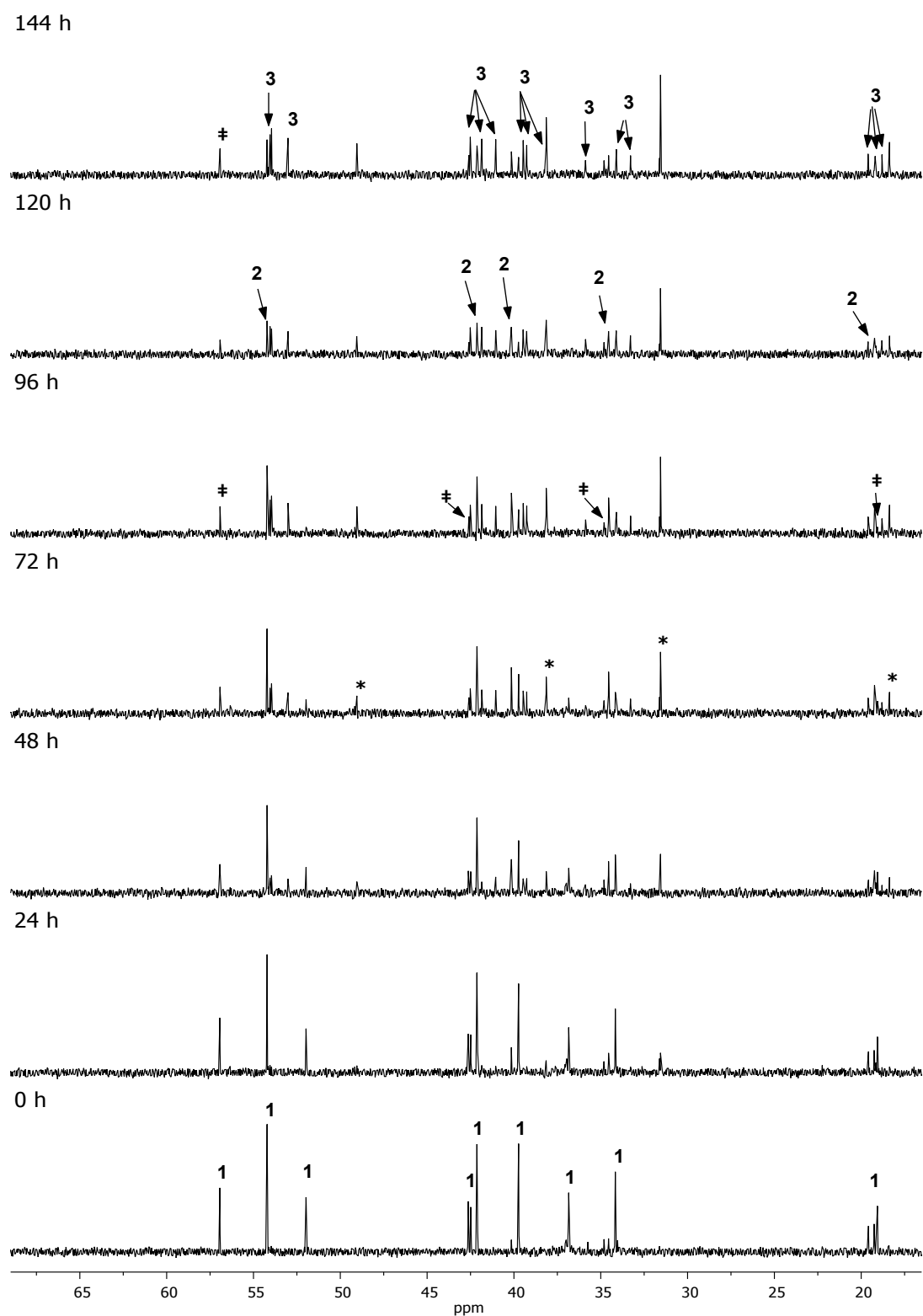


Figure S1f ^{13}C NMR spectra (125 MHz, 298 K, C_6D_6) of **1** heated to 50°C for the time specified. * = TMPH, ‡ = Cu-rich TMP-aggregate.

Additional characterisation of 2

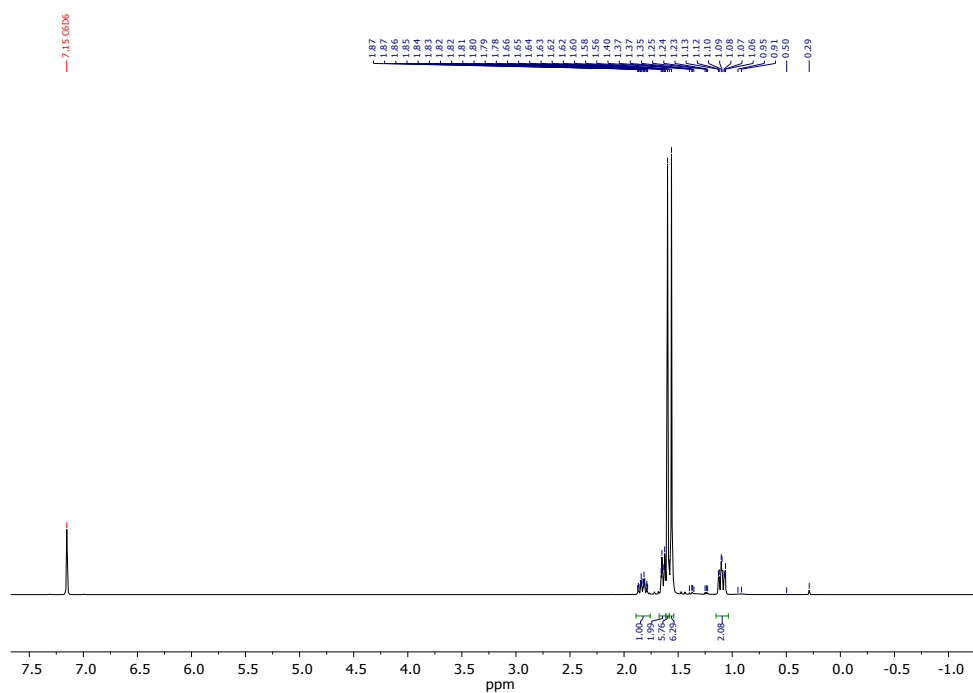


Figure S2a ¹H NMR spectrum of **2** (500 MHz, 298 K, C₆D₆).

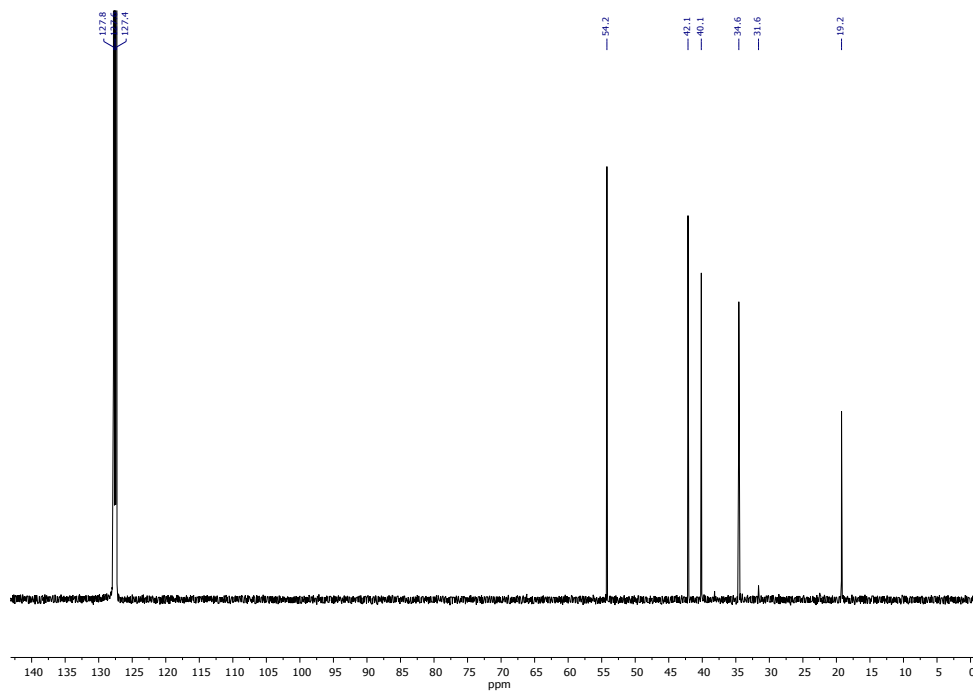
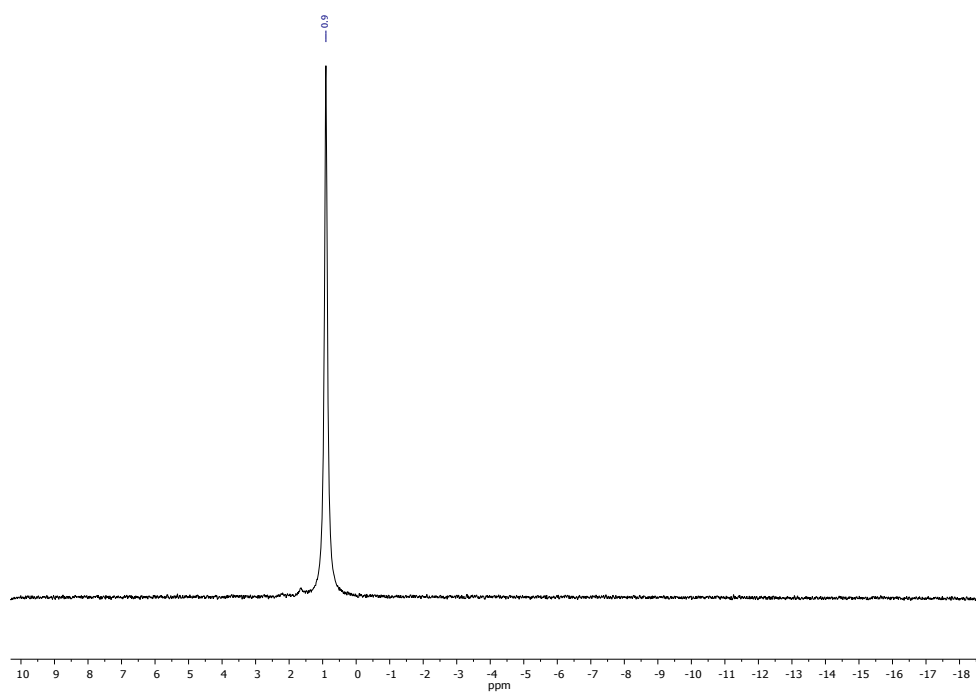


Figure S2b ¹³C NMR spectrum of **2** (125 MHz, 298 K, C₆D₆).



S2c ^7Li NMR spectrum of **2** (194 MHz, 298 K, C_6D_6).

Additional characterisation of 3

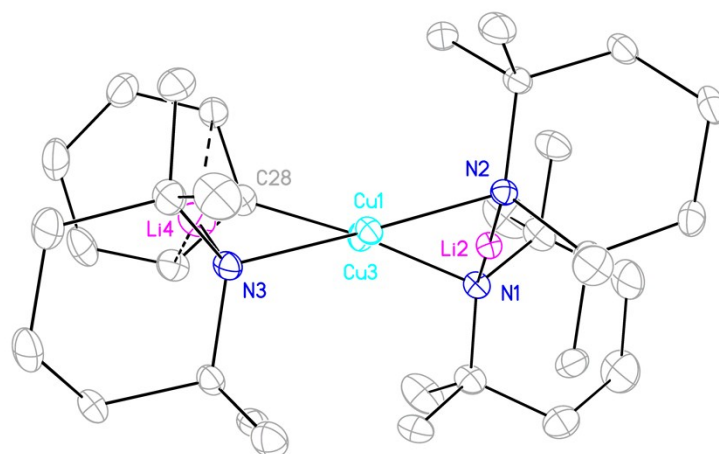


Figure S3a Side-view of **3**, showing deviation of the core metallacycle from planarity.

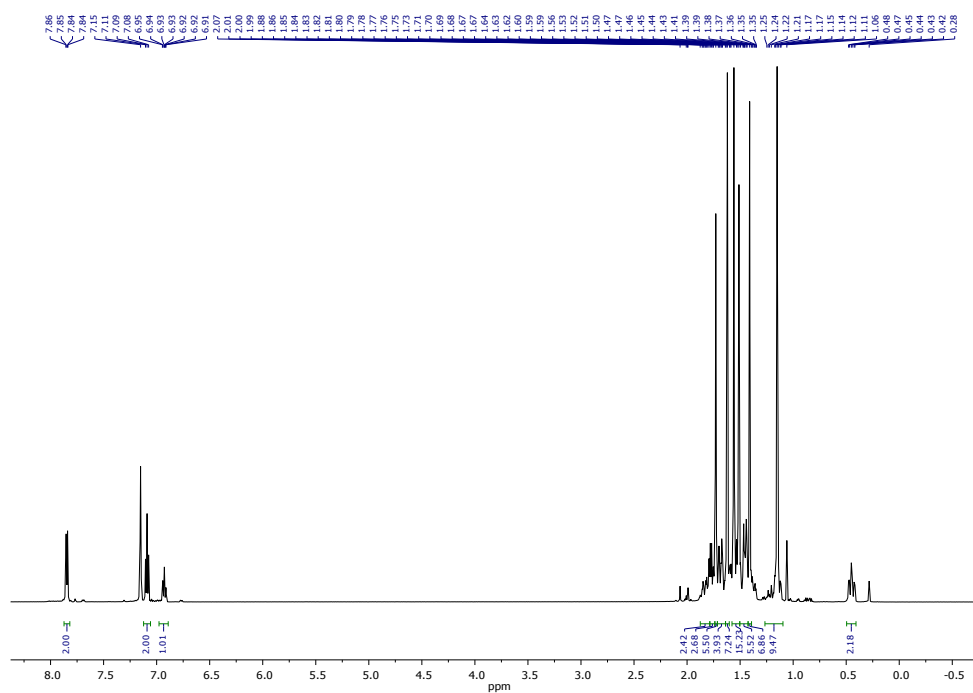


Figure S3b ^1H NMR spectrum of **3** (500 MHz, 298 K, C_6D_6).

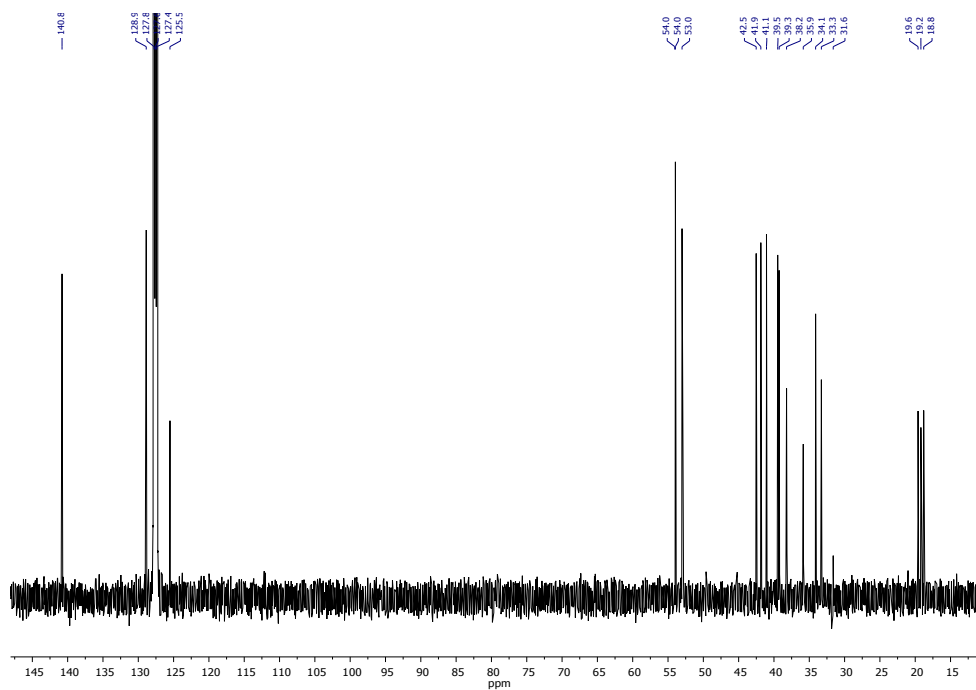


Figure S3c ^{13}C NMR spectrum of **3** (125 MHz, 298 K, C_6D_6).

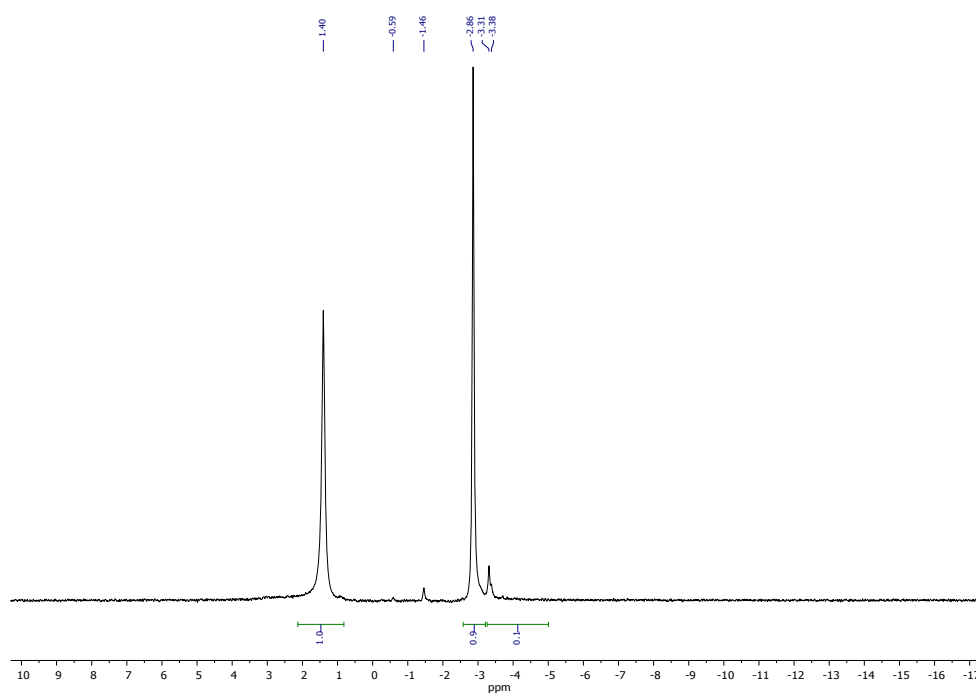


Figure S3d ^7Li NMR spectrum of **3** (194 MHz, 298 K, C_6D_6).

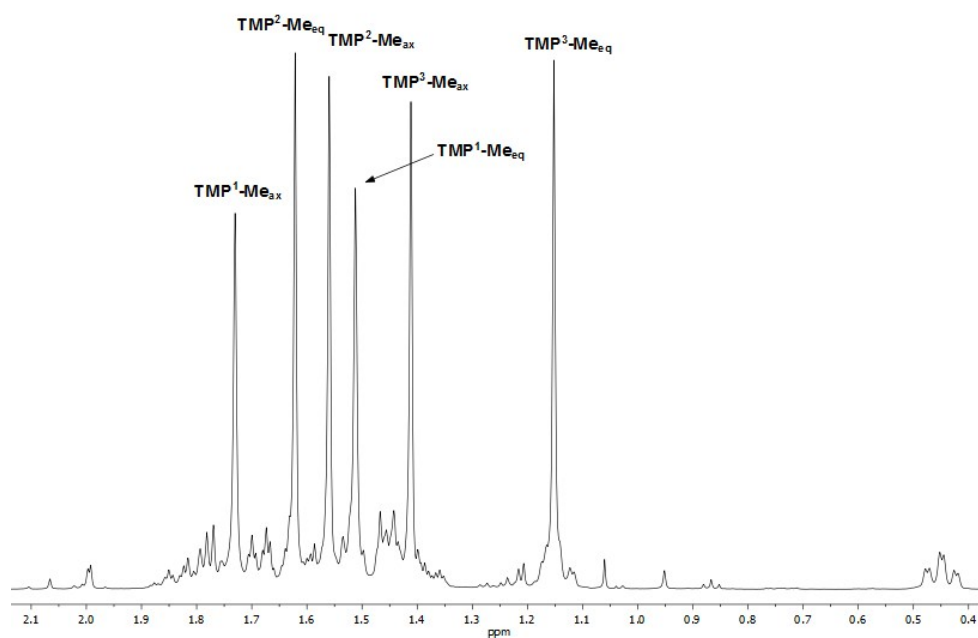


Figure S3e ^1H NMR spectra of **3** in C_6D_6 (at 298 K); expansions of aliphatic with TMP-Me groups annotated.

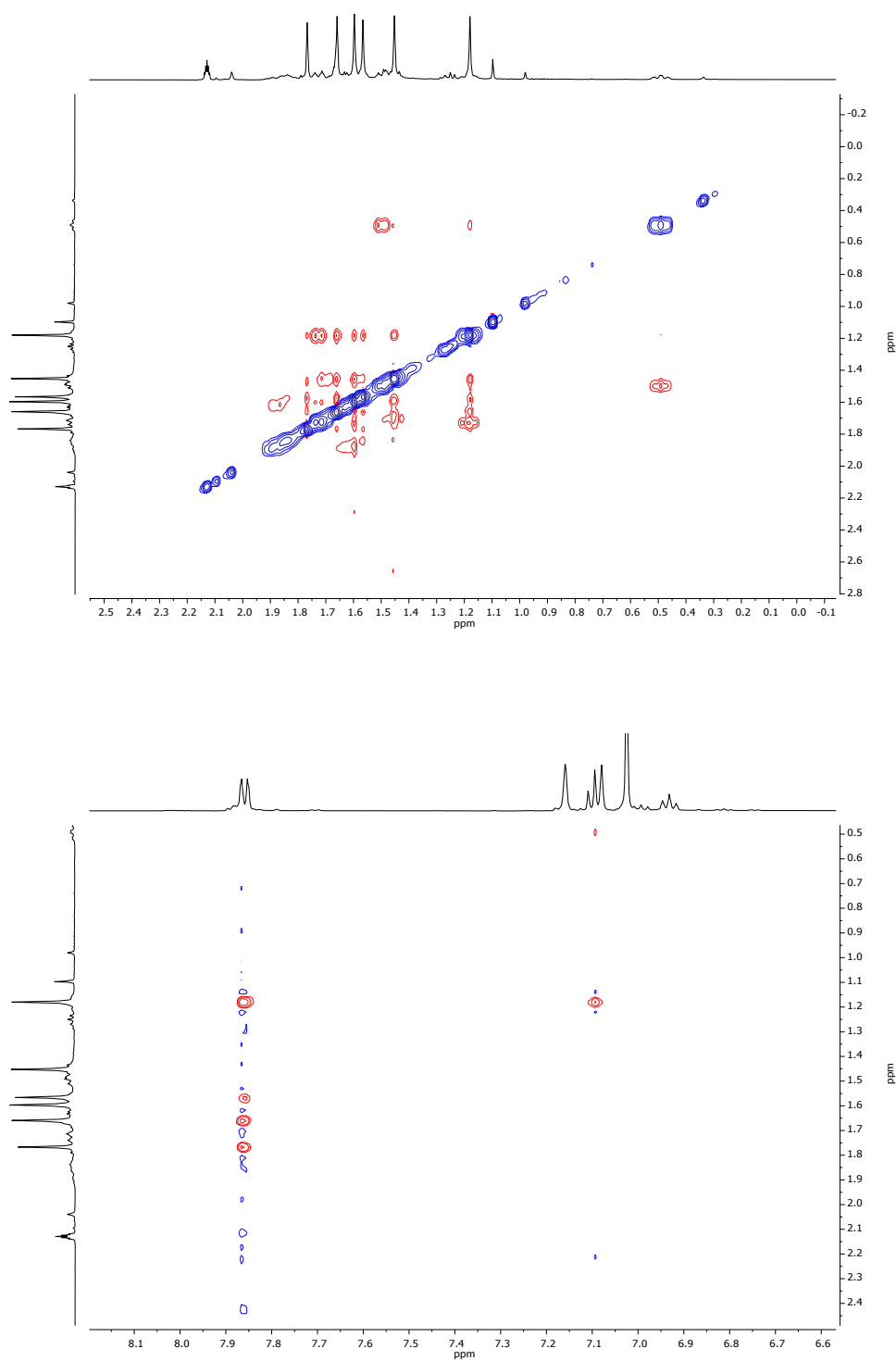


Figure S3f ^1H , ^1H -NOESY spectra of **3** (500 MHz, 263 K, C_7D_8 , $\tau = 0.6$ s). The observation of NOEs to the *o*-Ph hydrogens from both axial and equatorial Me-groups of TMP^1 but only the equatorial groups of TMP^2 and TMP^3 is consistent with TMP^1 lying *endo*.

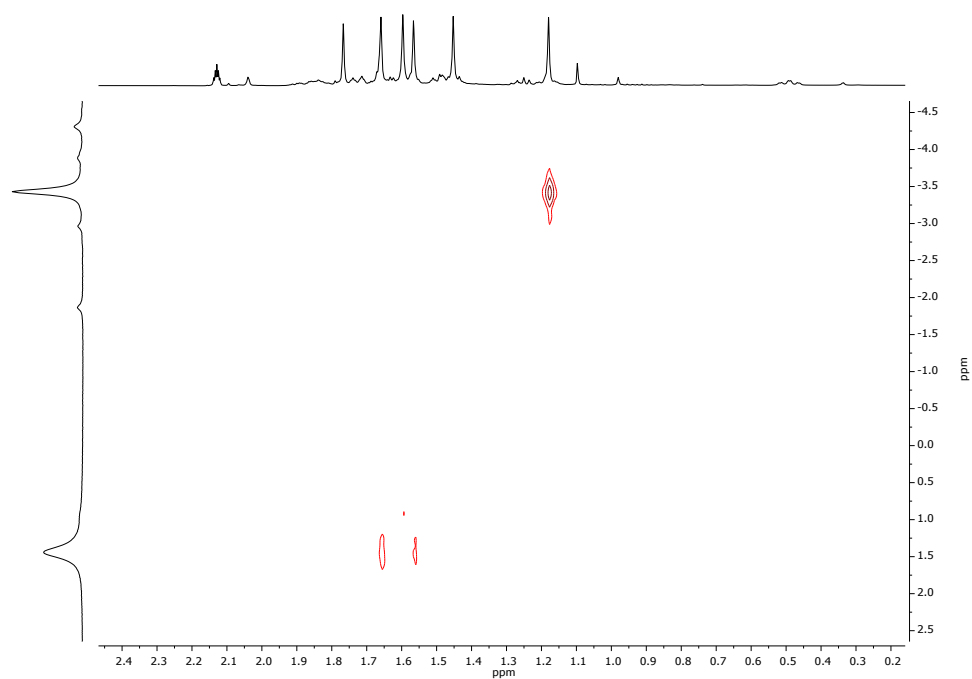


Figure S3g ^1H , ^7Li -HOESY spectrum of **3** (500 MHz, 263 K, C_7D_8 ; $\tau = 0.05$ s).

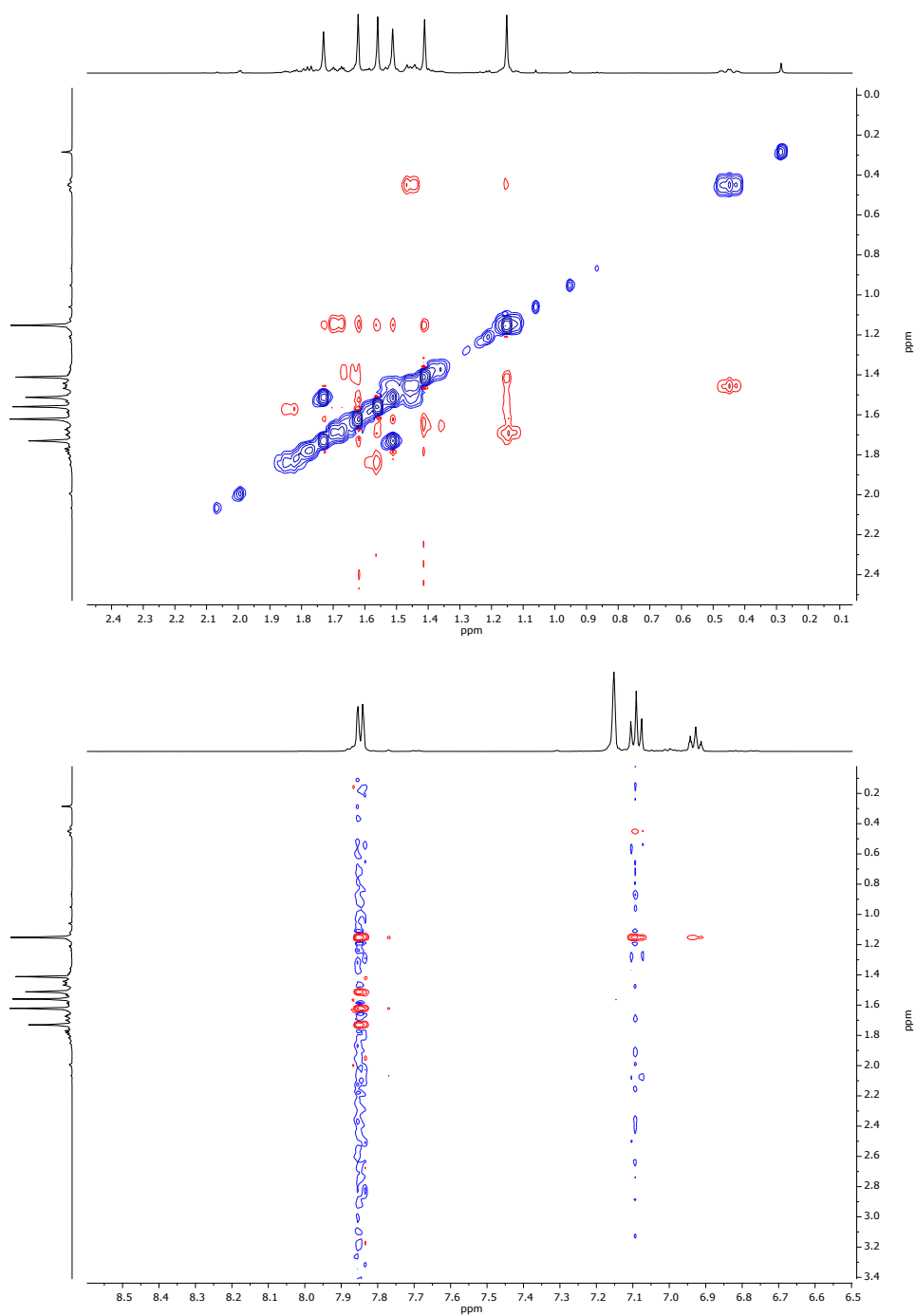


Figure S3h ^1H , ^1H -NOESY spectra of **3** (500 MHz, 298 K, C_6D_6 , $\tau = 0.6$ s).

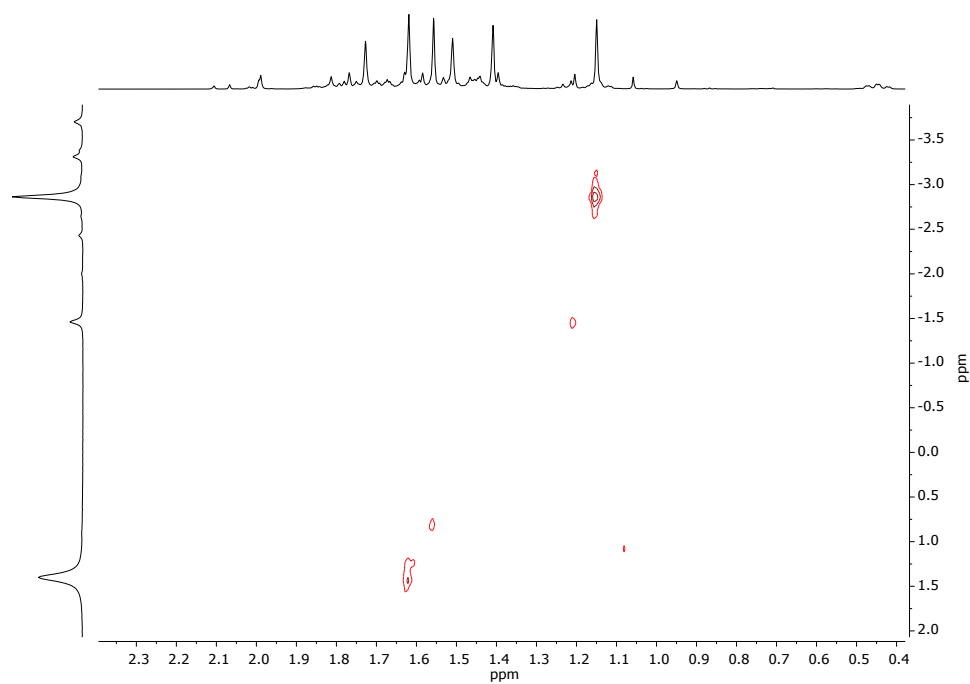


Figure S3i ^1H , ^7Li -HOESY spectrum of **3** (500 MHz, 298 K, C_6D_6 , $\tau = 0.05$ s).

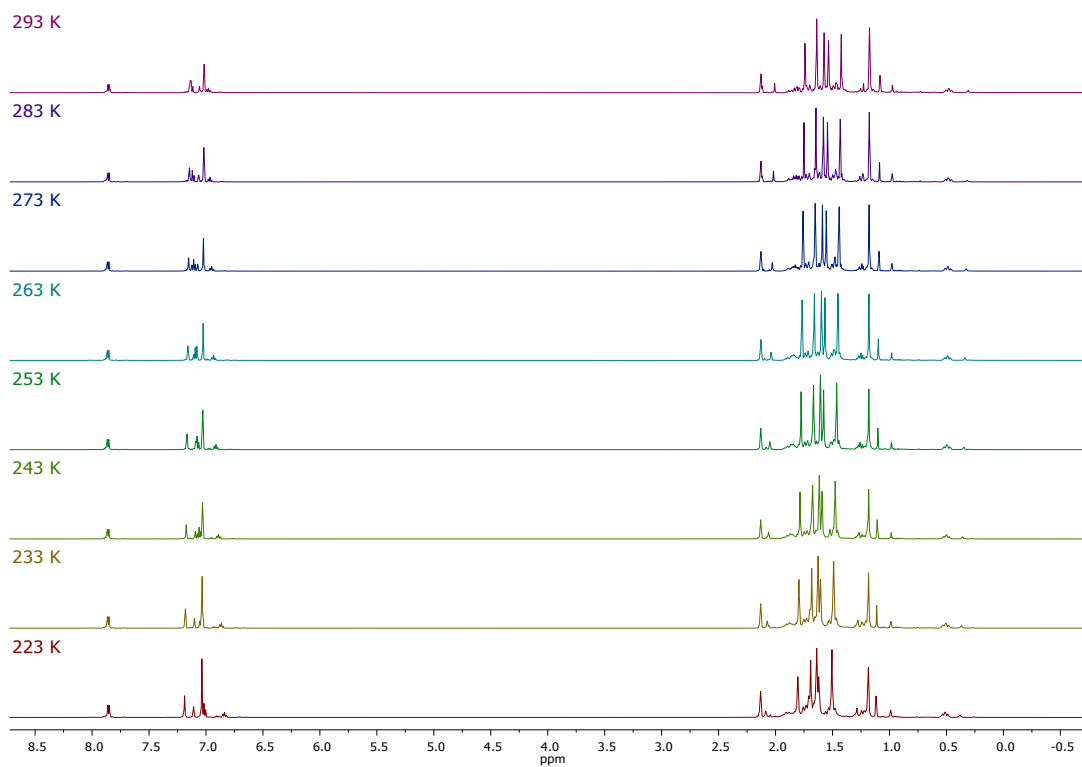


Figure S3j Variable temperature ^1H NMR spectra of **3** (500 MHz, T (specified), C_7D_8).

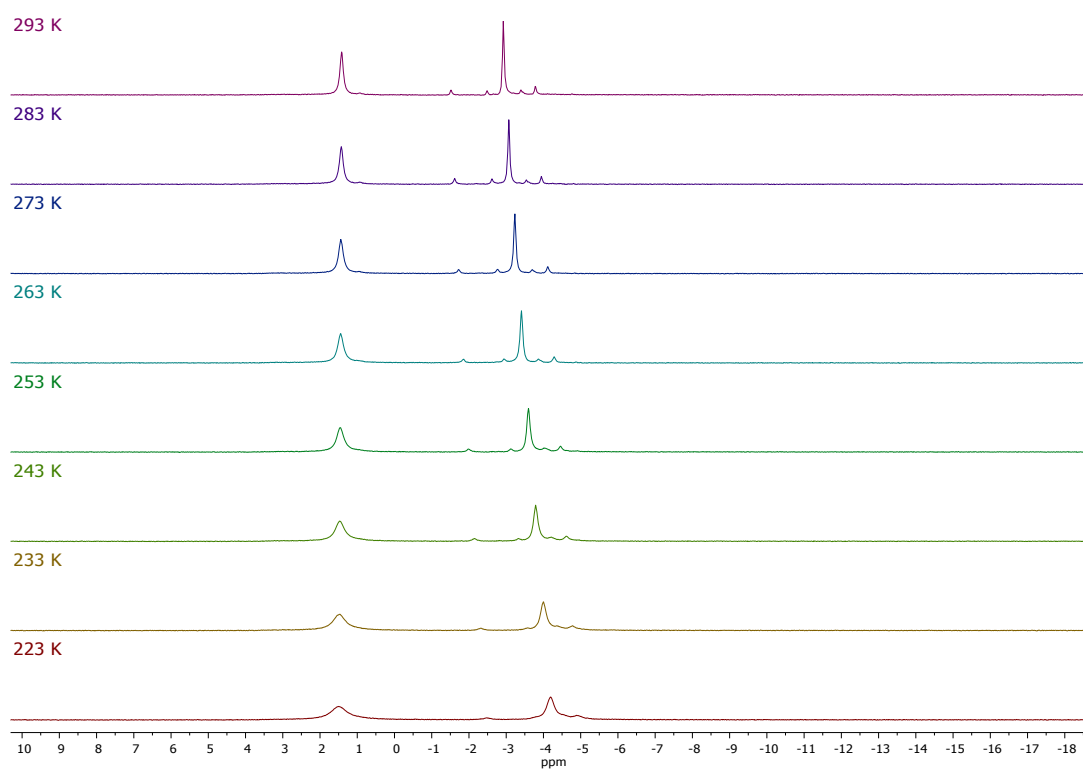


Figure S3k Variable temperature ^7Li NMR spectra of **3** (194 MHz, T (specified), C_7D_8).

Additional characterisation of 4

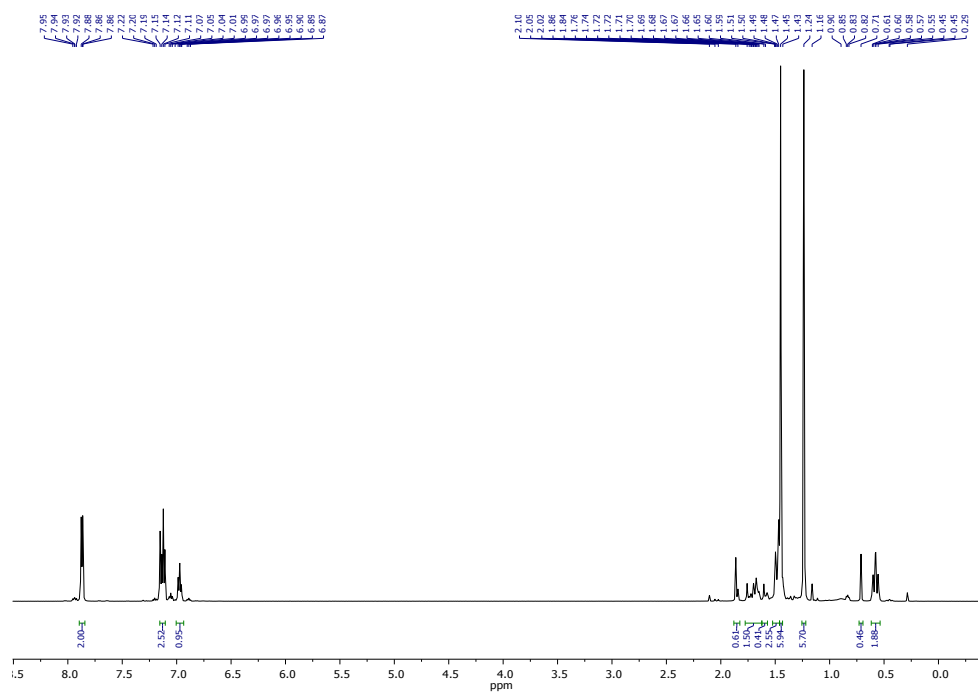


Figure S4a ¹H NMR spectrum of **4** (500 MHz, 298 K, C₆D₆).

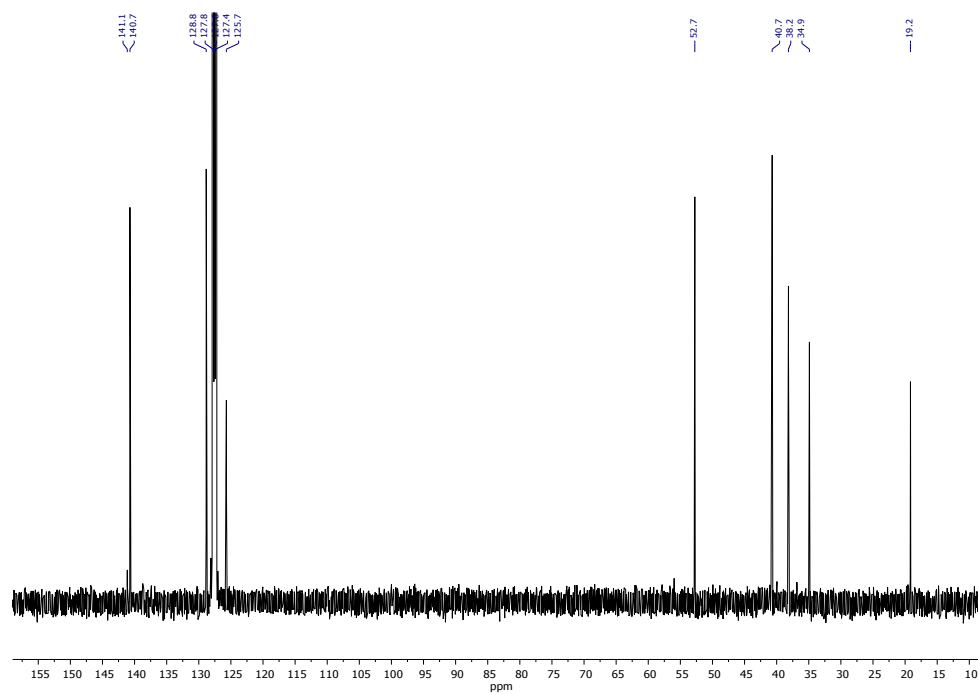


Figure S4b ¹³C NMR spectrum **4** (125 MHz, 298 K, C₆D₆).

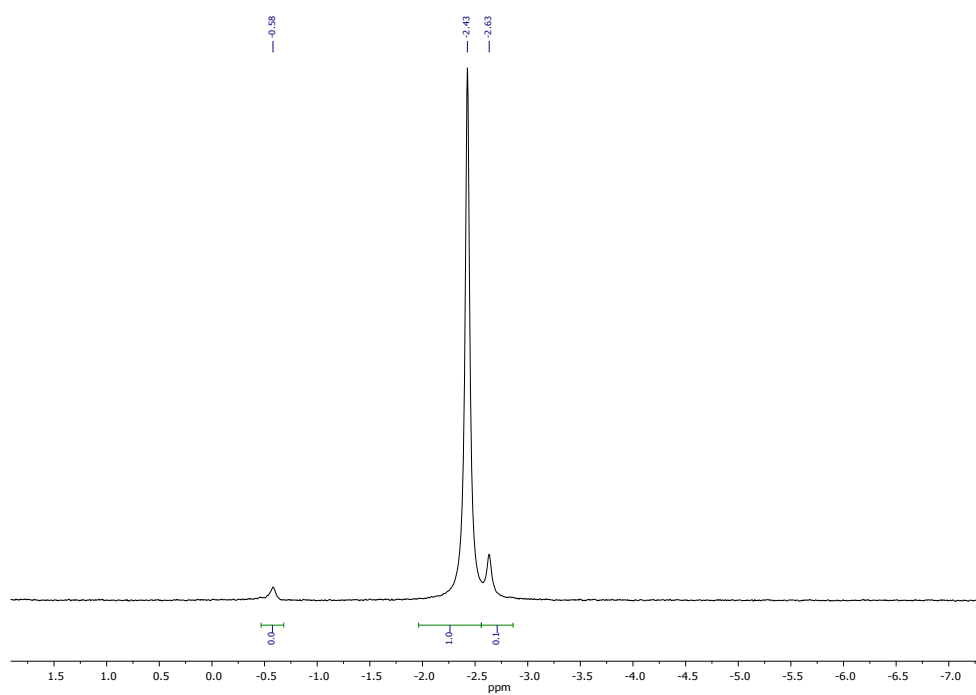


Figure S4c ^7Li NMR spectrum of **4** (194 MHz, 298 K, C_6D_6).

Additional characterisation of **5**

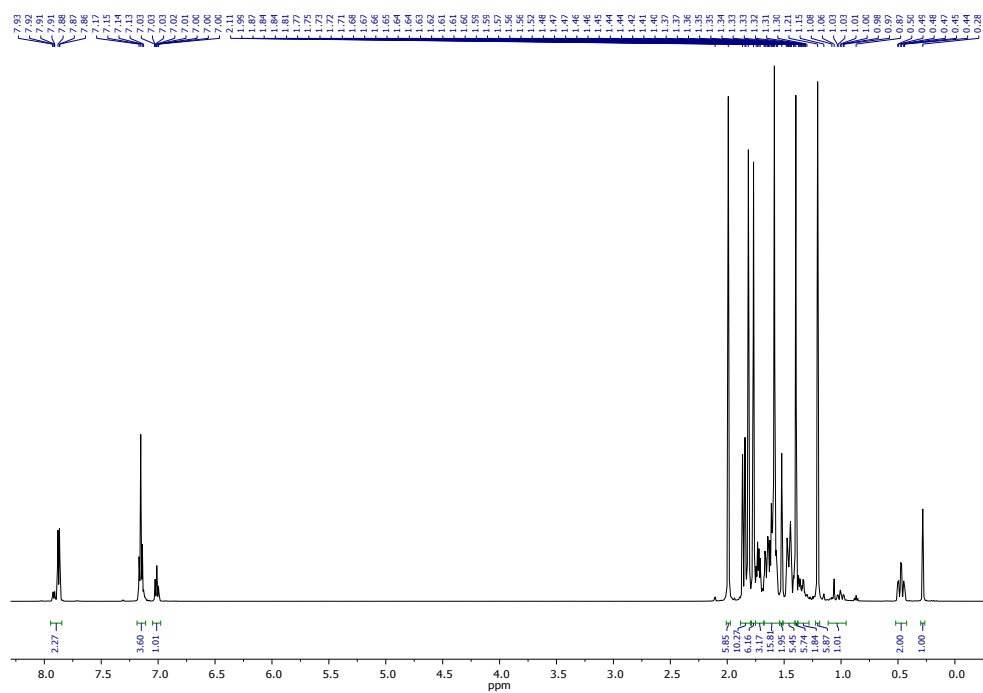


Figure S5a ¹H NMR spectrum of **5** (500 MHz, 298 K, C₆D₆).

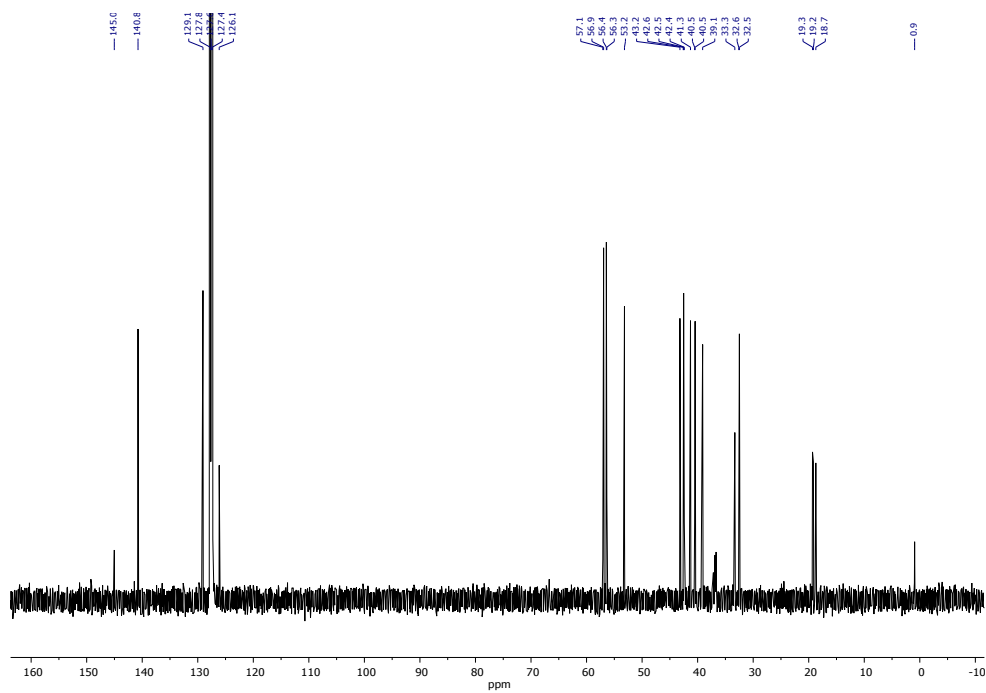


Figure S5b ¹³C NMR spectrum of **5** (125 MHz, 298 K, C₆D₆).

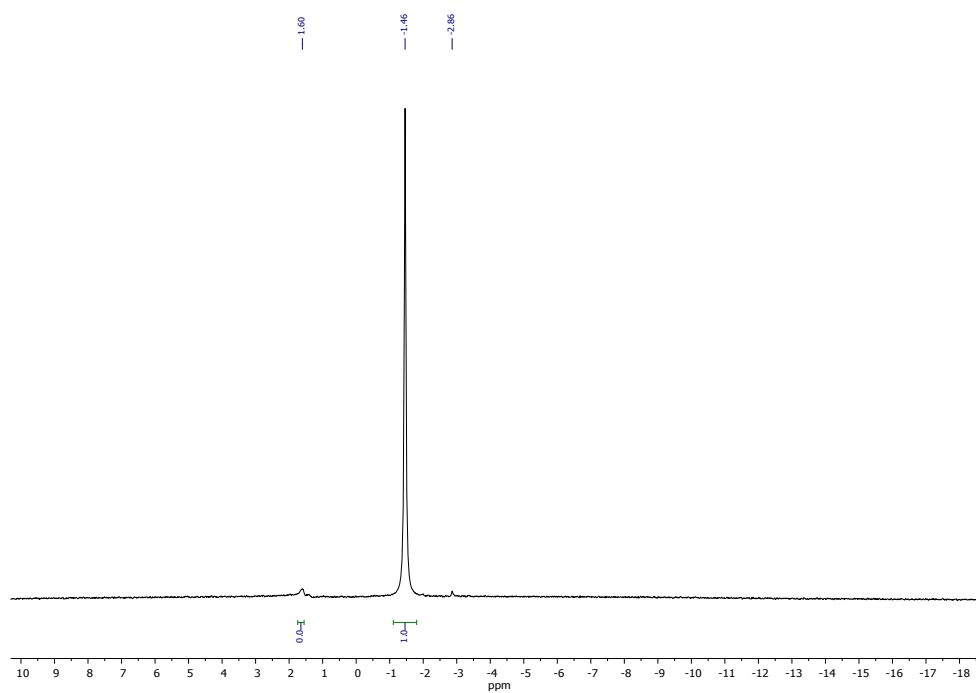


Figure S5c ^7Li NMR spectrum of **5** (194 MHz, 298 K, C_6D_6).

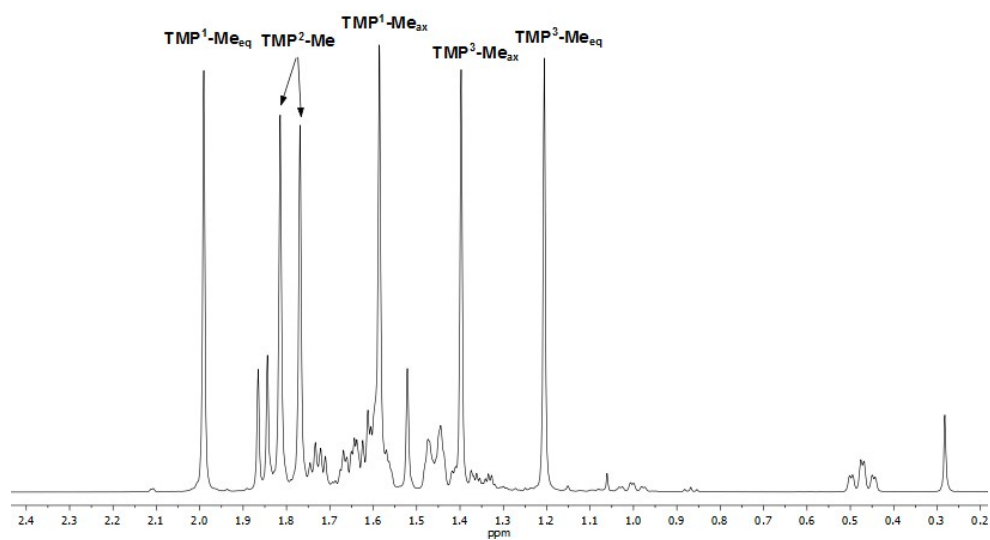


Figure S5d ^1H NMR spectrum of **5** (500 MHz, 298 K, C_6D_6); expansion of aliphatic region.

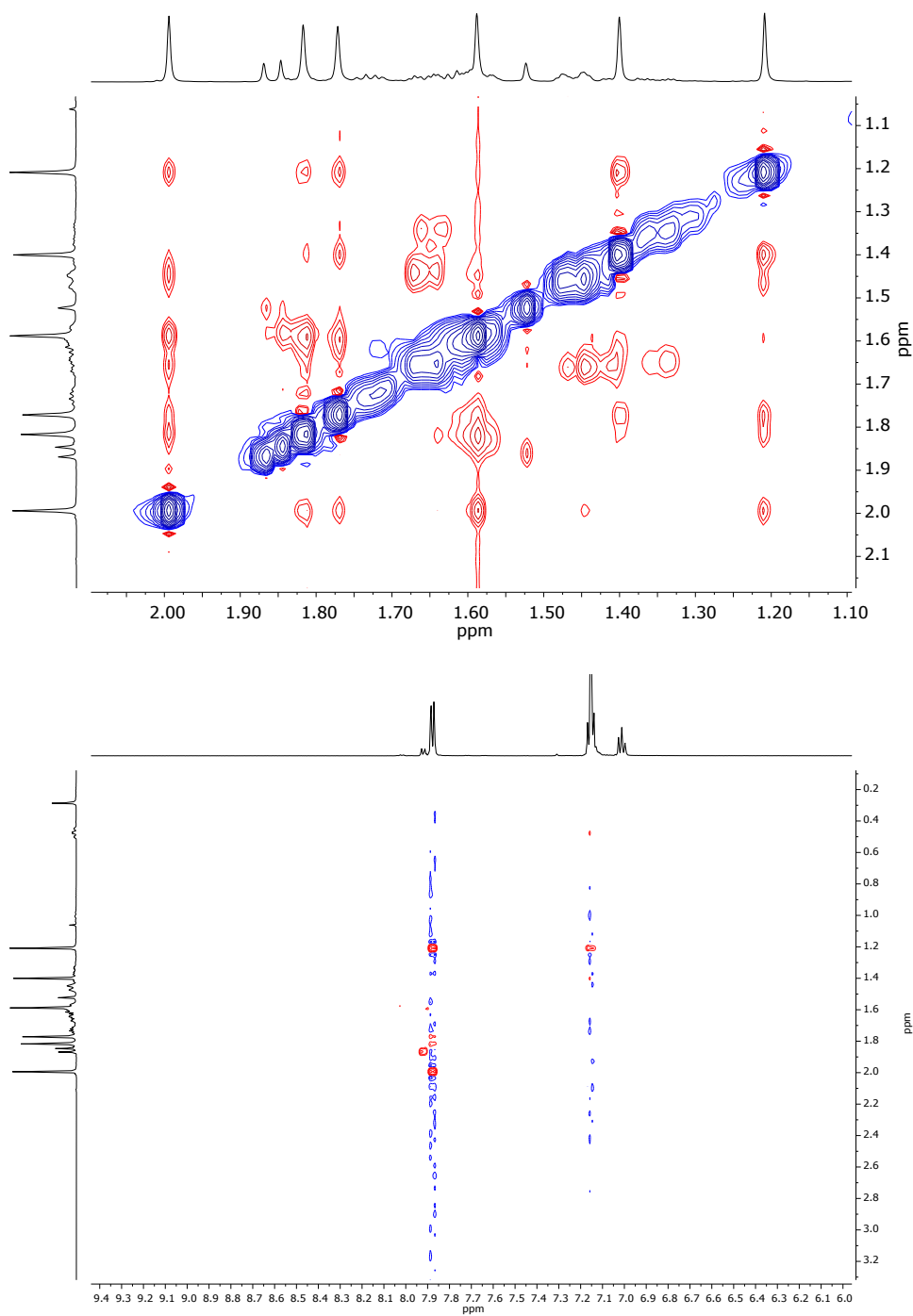


Figure S5e ^1H , ^1H -NOESY spectra of **5** (500 MHz, 298 K, C_6D_6 , $\tau = 0.6$ s).

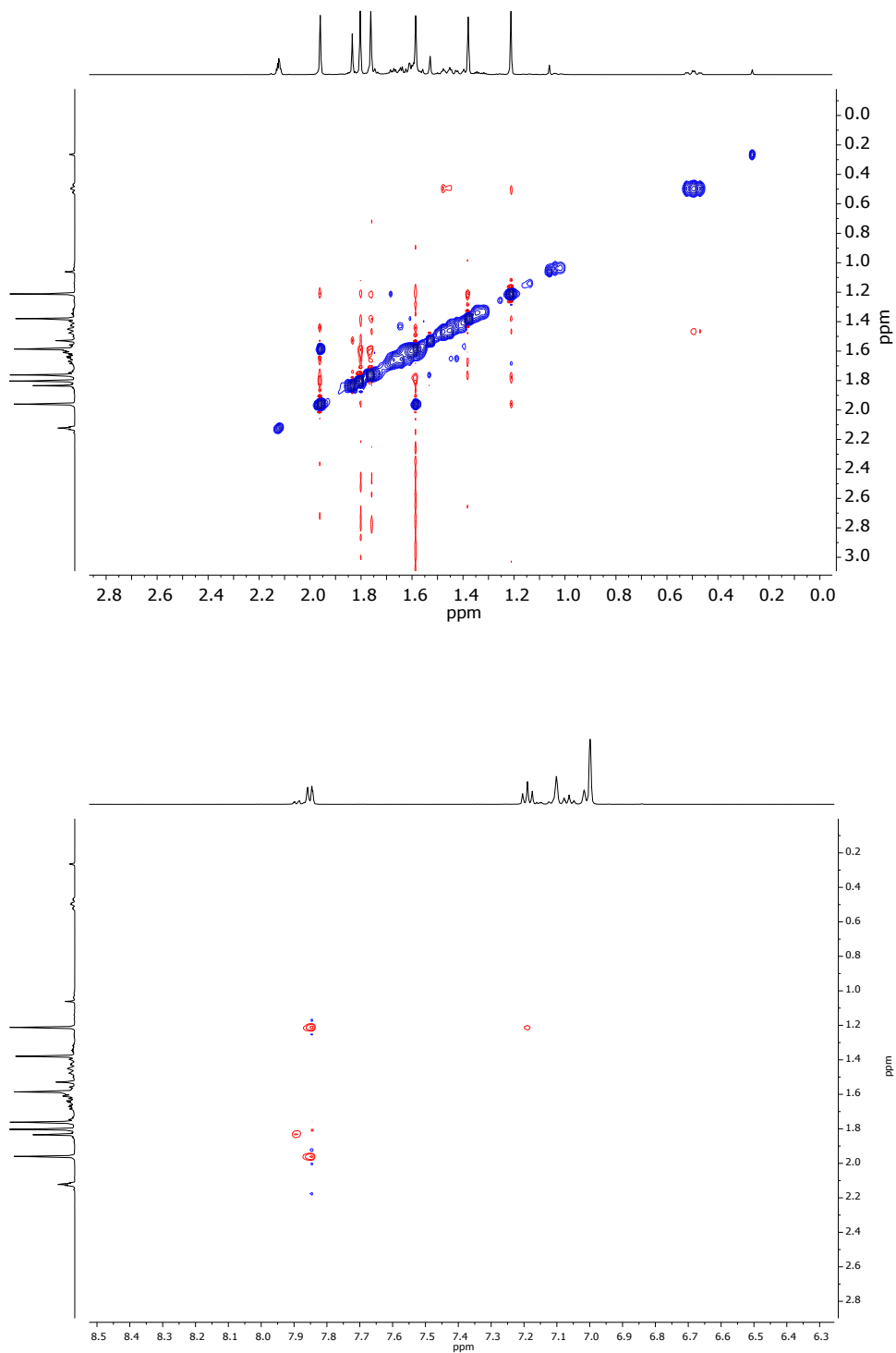


Figure S5f ^1H , ^1H -NOESY spectra of **5** (500 MHz, 353 K, C_7D_8 , $\tau = 0.6$ s).

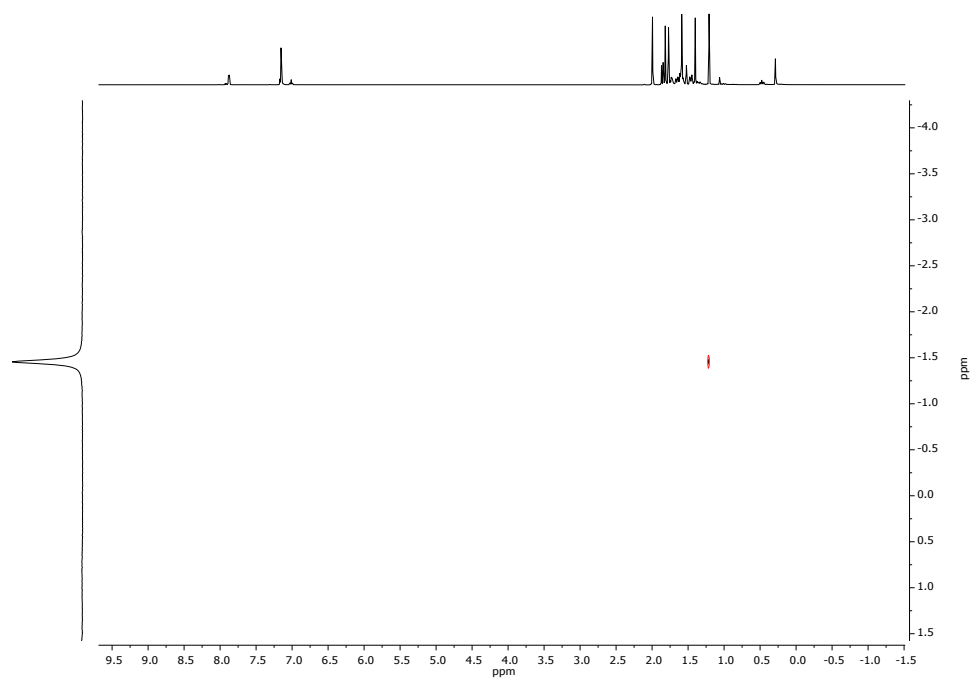


Figure S5g $^1\text{H}, ^7\text{Li}$ -HOESY spectrum of **5** (500 MHz, 298 K, C_6D_6 , $\tau = 0.1$).

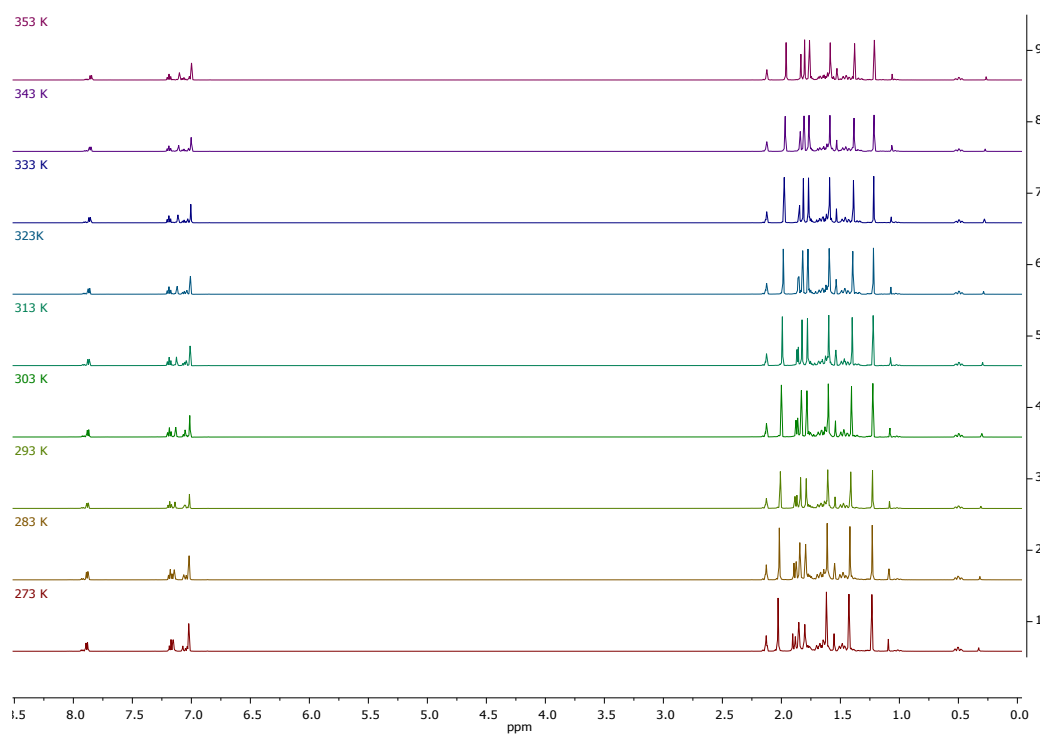


Figure S5h Variable temperature ^1H NMR spectra of **5** (500 MHz, T (specified), C_7D_8).

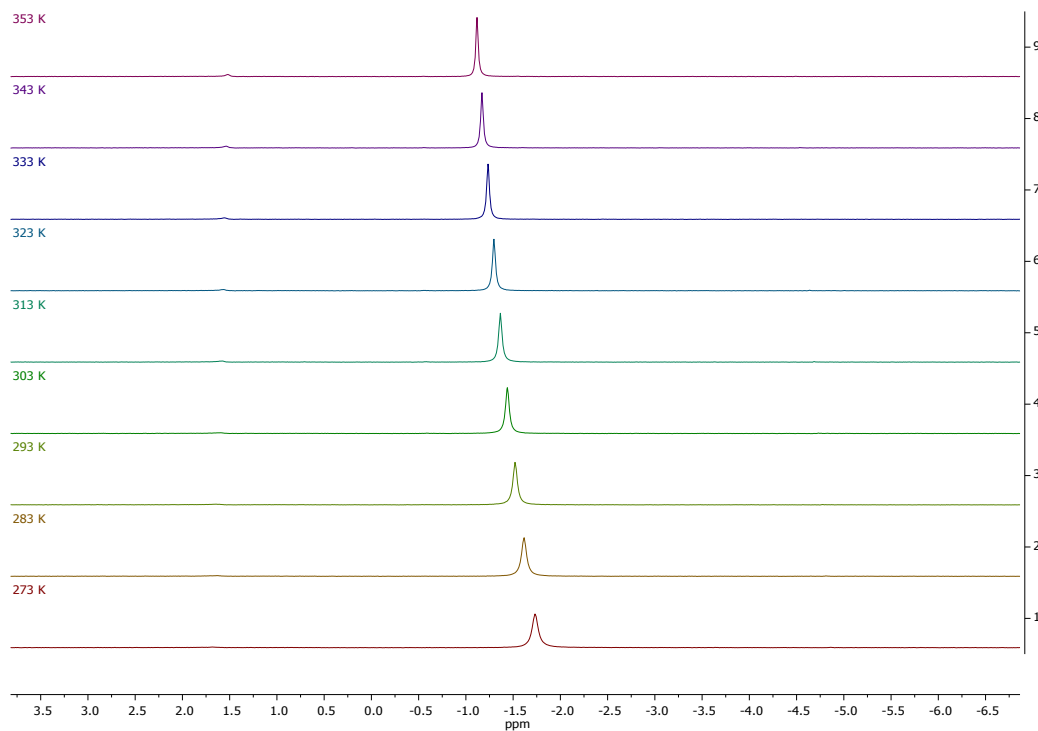


Figure S5i Variable temperature ^7Li NMR spectra of **5** (194 MHz, T (specified), C_7D_8).

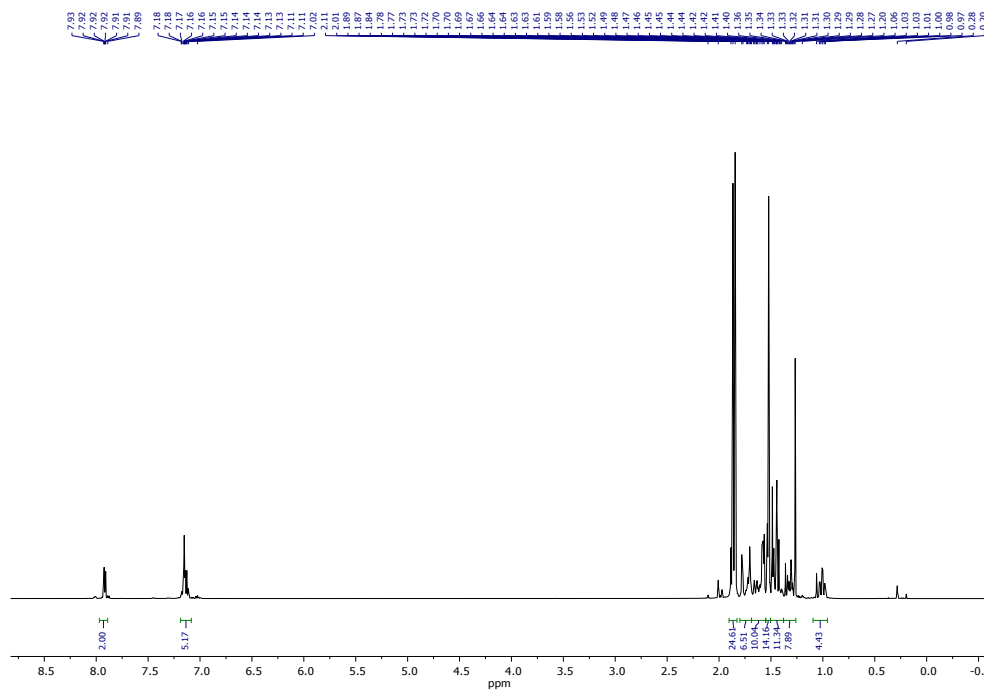


Figure S5j ^1H NMR spectrum (500 MHz, 298 K, C_6D_6) on a 1:1 mixture of **5** and $t\text{BuOCu}$, heated to 50°C for 24 h (*cf.* Fig. S6a).

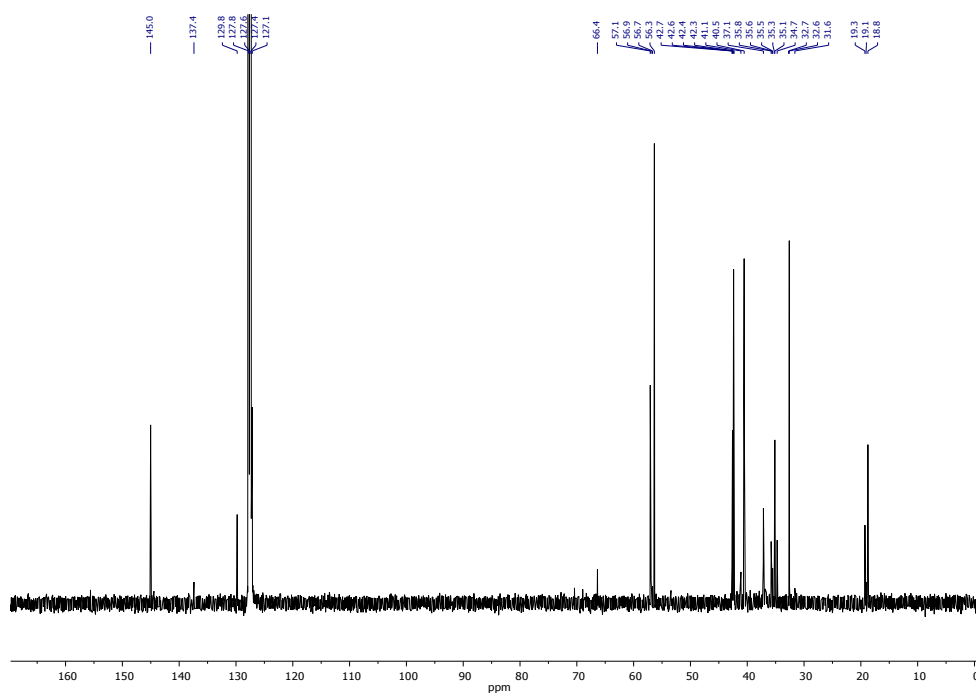


Figure S5k ^{13}C NMR spectrum (125 MHz, 298 K, C_6D_6) on a 1:1 mixture of **5** and $t\text{BuOCu}$, heated to 50°C for 24 h (cf. Fig. S6b).

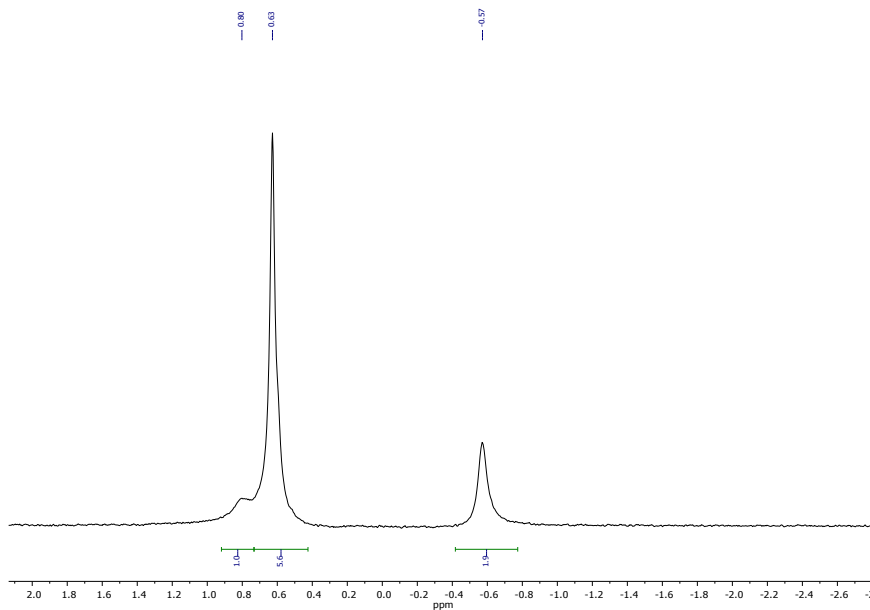


Figure S5l ^7Li NMR spectrum (125 MHz, 298 K, C_6D_6) on a 1:1 mixture of **5** and $t\text{BuOCu}$, heated to 50°C for 24 h. The major resonance at δ 0.63 ppm is due to $t\text{BuOLi}$.¹

¹ J. F. Allan, R. Nassar, E. Specht, A. Beatty, N. Calin and K. Henderson, *J. Am. Chem. Soc.*, 2004, **126**, 484-485.

Additional Characterisation of **6**

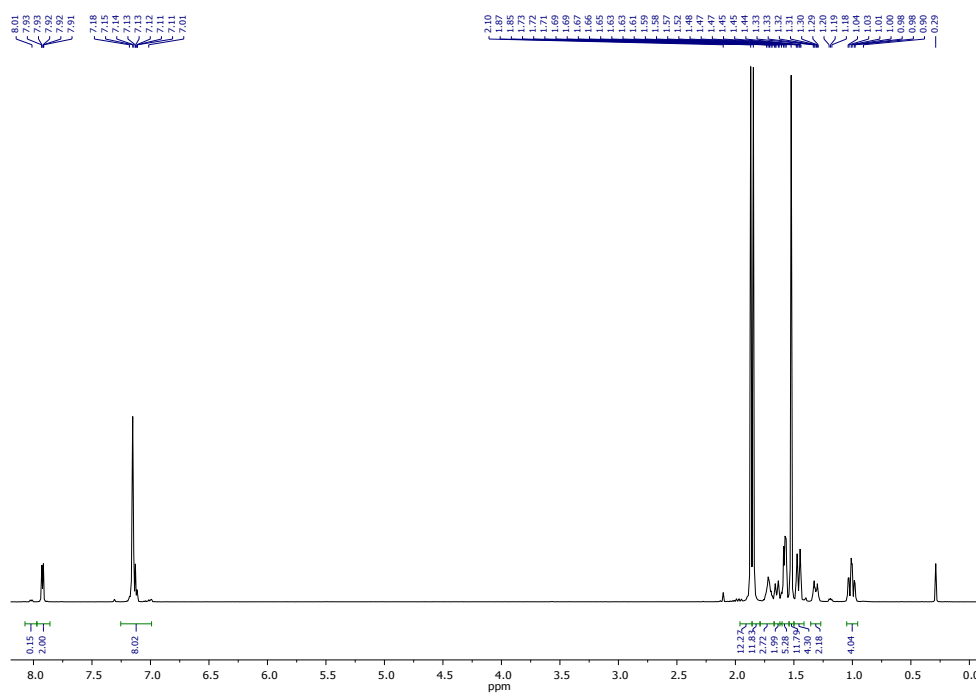


Figure S6a. ¹H NMR spectrum of **6** (500 MHz, 298 K, C₆D₆).

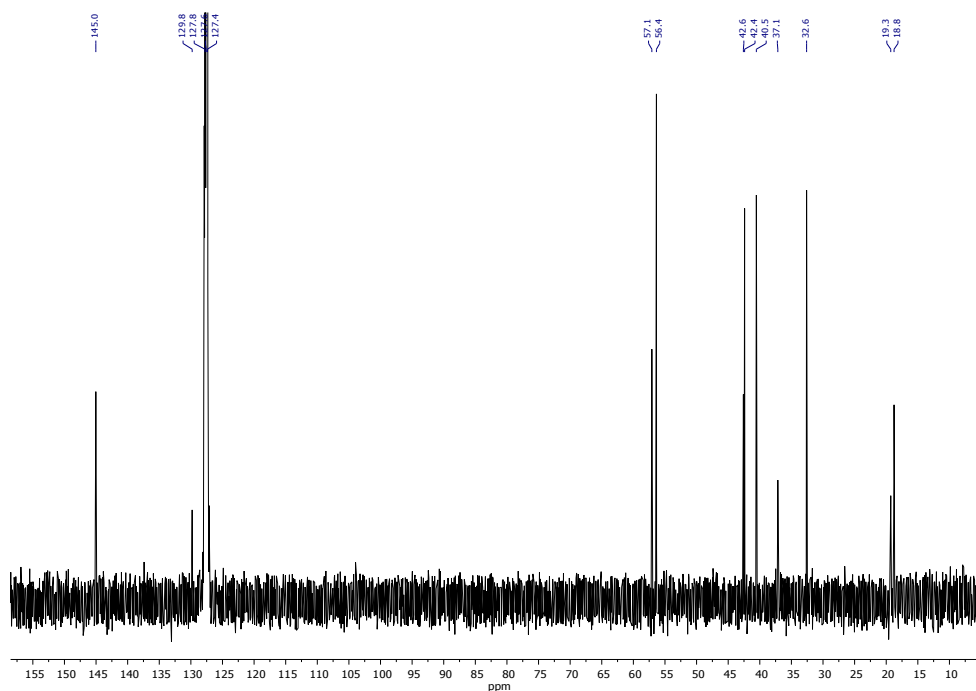


Figure S6b. ¹³C NMR spectrum of **6** (125 MHz, 298 K, C₆D₆).

Additional characterisation of 7

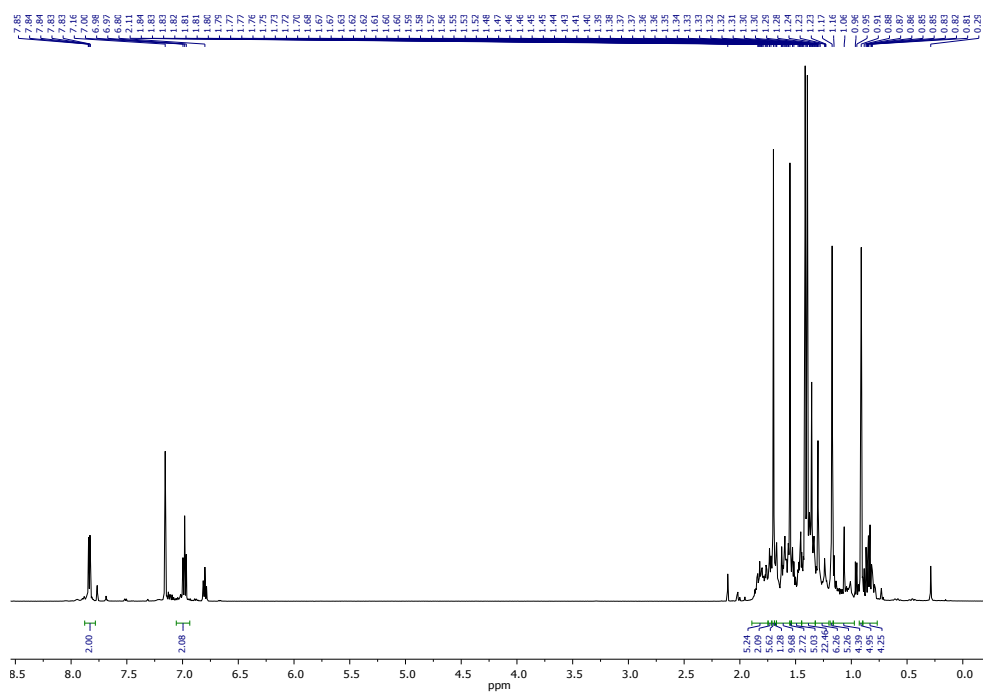


Figure S7a ¹H NMR spectrum of 7 (500 MHz, 298 K, C₆D₆).

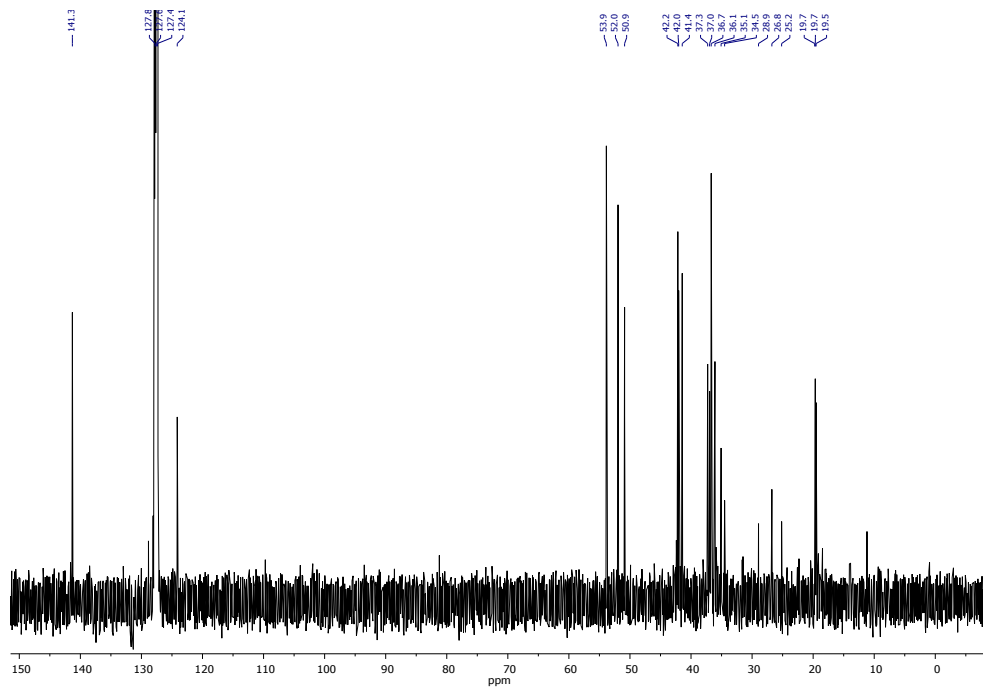


Figure S7b ¹³C NMR spectrum of 7 (125 MHz, 298 K, C₆D₆).

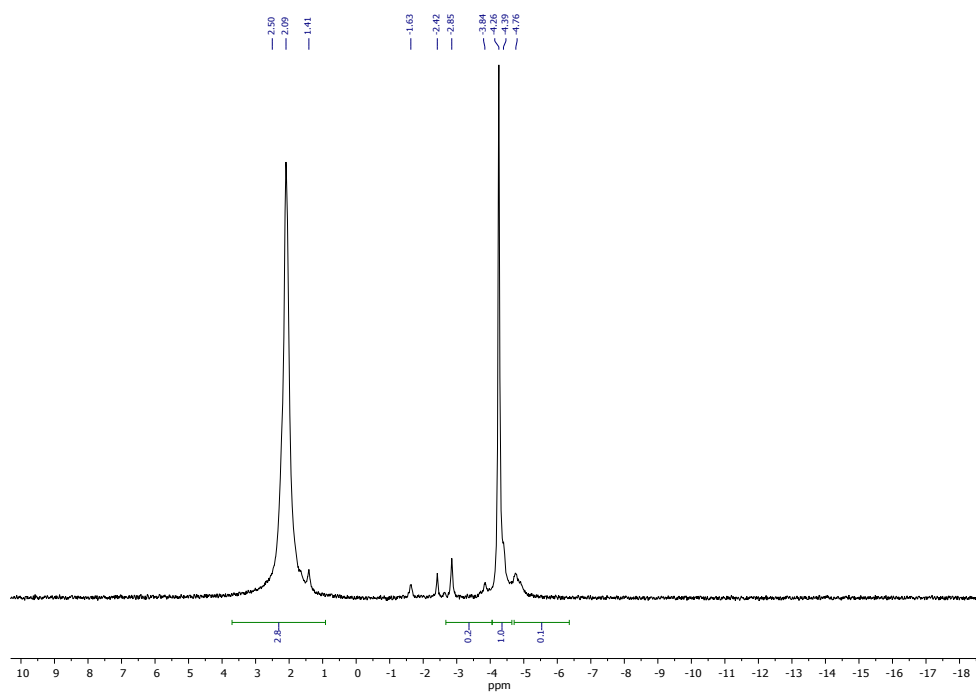


Figure S7c ^7Li NMR spectrum of **7** (194 MHz, 298 K, C_6D_6).

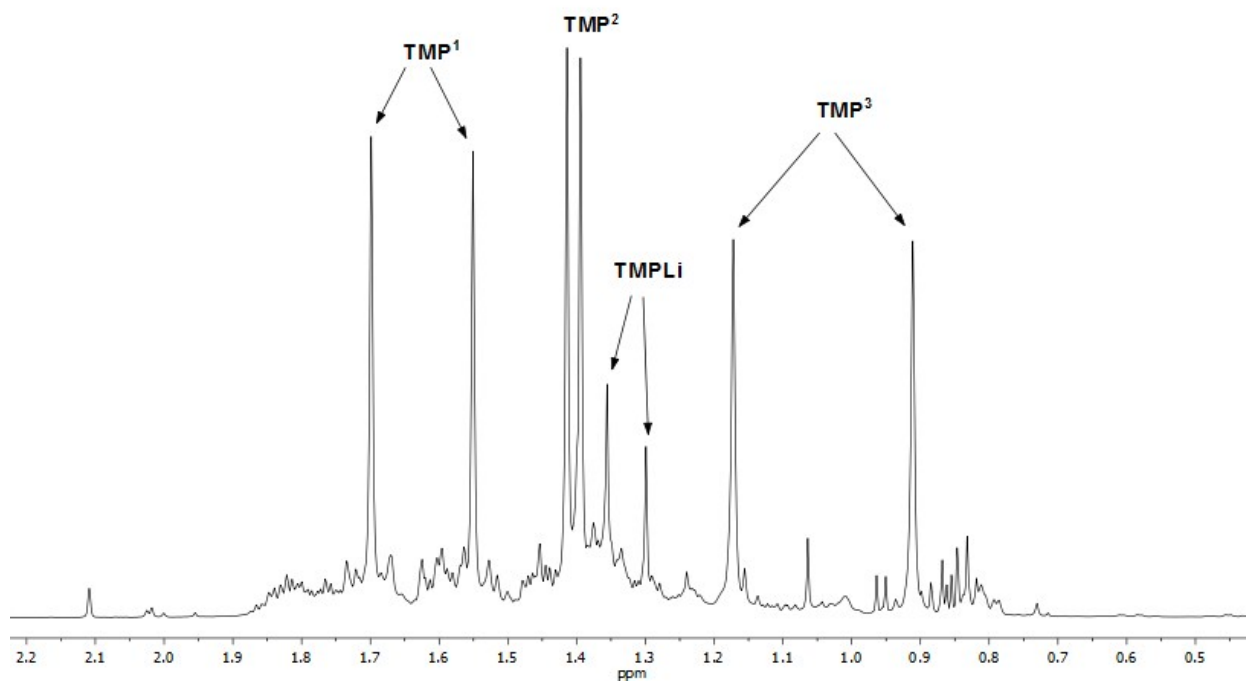


Figure S7d ^1H NMR spectrum of **7** (500 MHz, 298 K, C_6D_6).

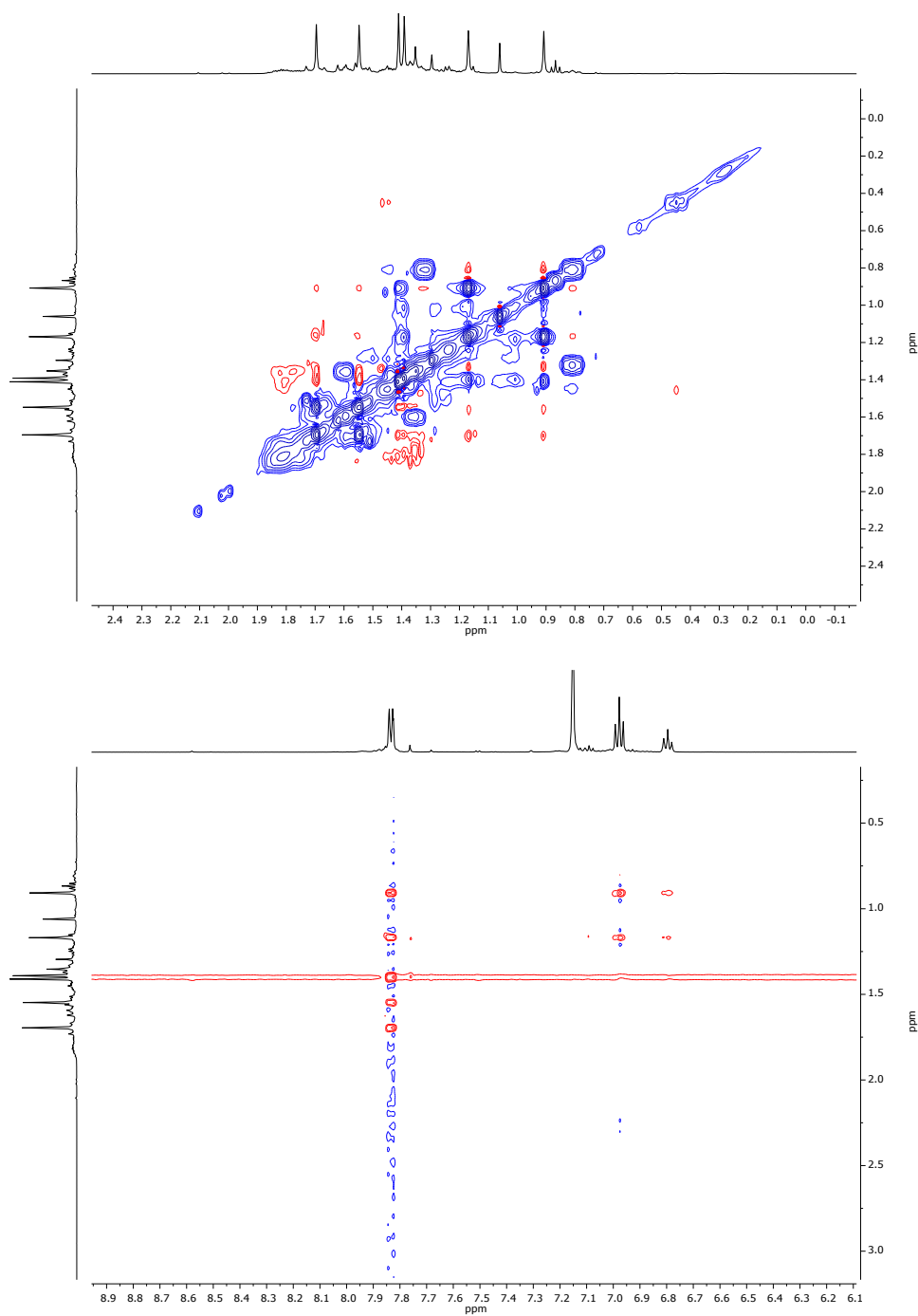


Figure S7e ^1H , ^1H -NOESY spectrum of **7** (500 MHz, 298 K, C_6D_6 , $\tau = 0.6$ s).

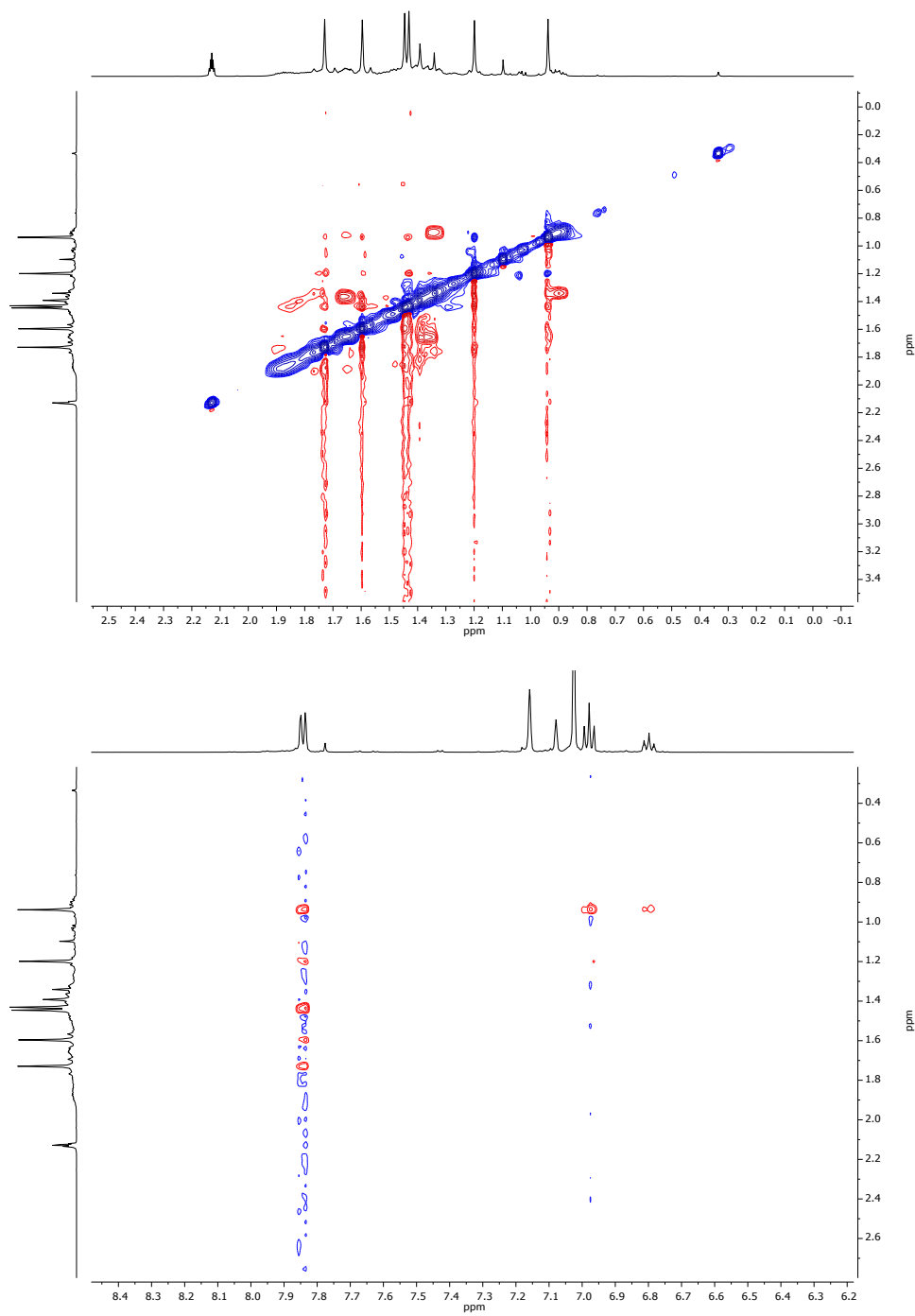


Figure S7f ^1H , ^1H -NOESY spectra of **7** (500 MHz, 263 K, C_7D_8 , $\tau = 0.6$ s).

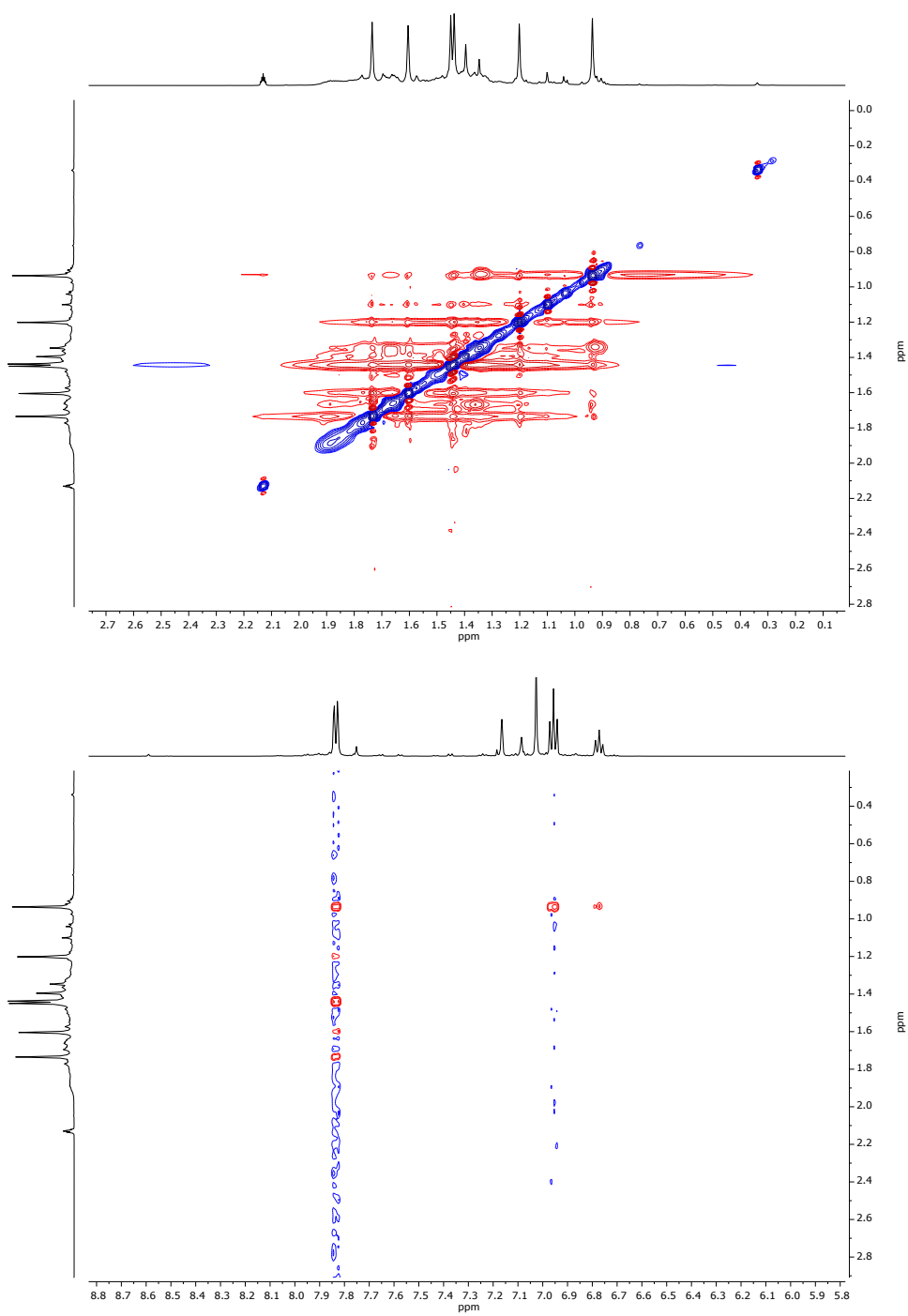


Figure S7g ^1H , ^1H -NOESY spectrum of **7** (500 MHz, 253 K, C_7D_8 , $\tau = 0.6$ s).

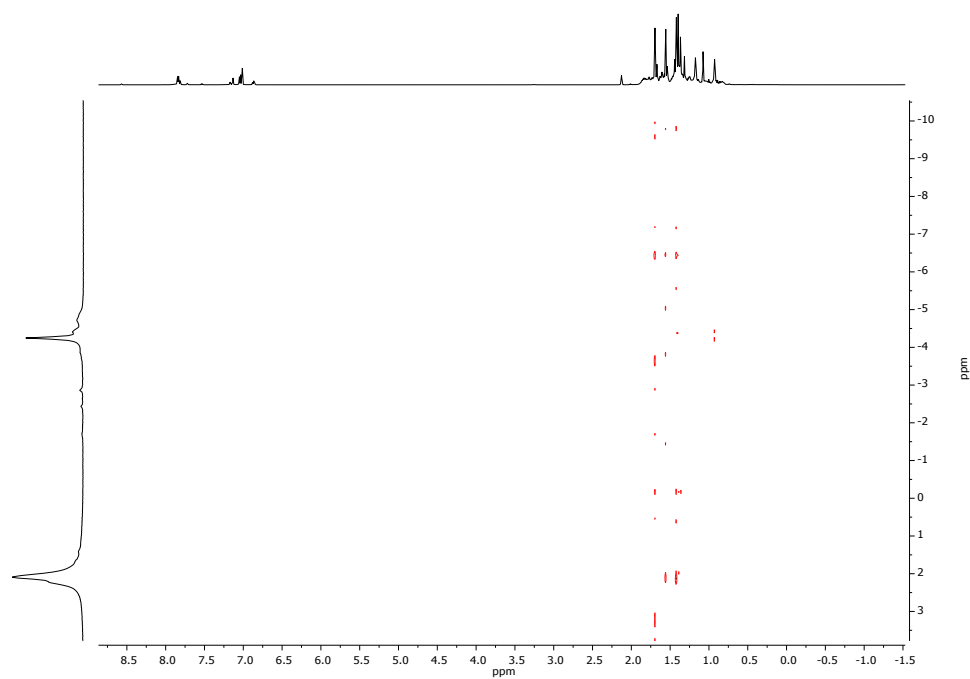


Figure S7h $^1\text{H}, ^7\text{Li}$ -HOESY spectrum of **7** (500 MHz, 298 K, C_6D_6 , $\tau = 0.05$ s).

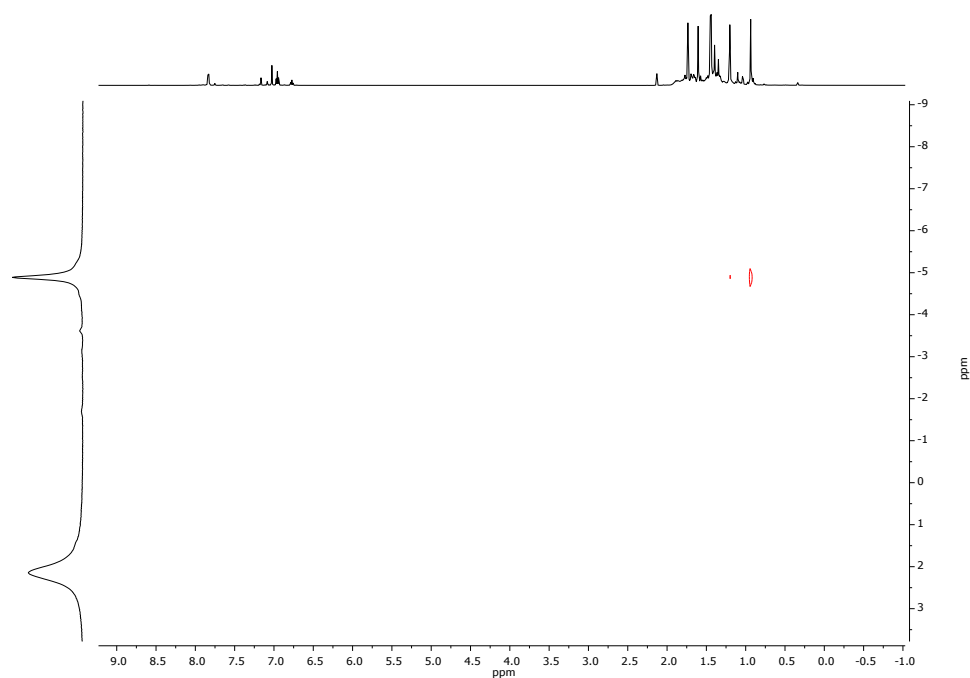


Figure S7i $^1\text{H}, ^7\text{Li}$ -HOESY spectrum of **7** (500 MHz, 253 K, C_7D_8).

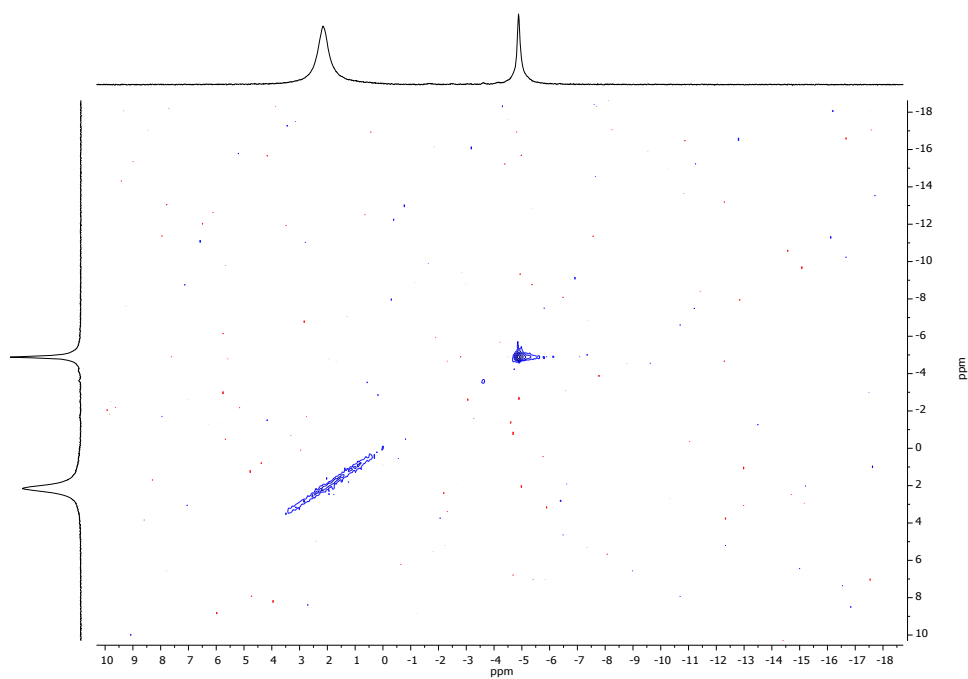


Figure S7j ${}^7\text{Li}$, ${}^7\text{Li}$ -NOESY spectrum of 7 (194 MHz, 253 K, C_7D_8).

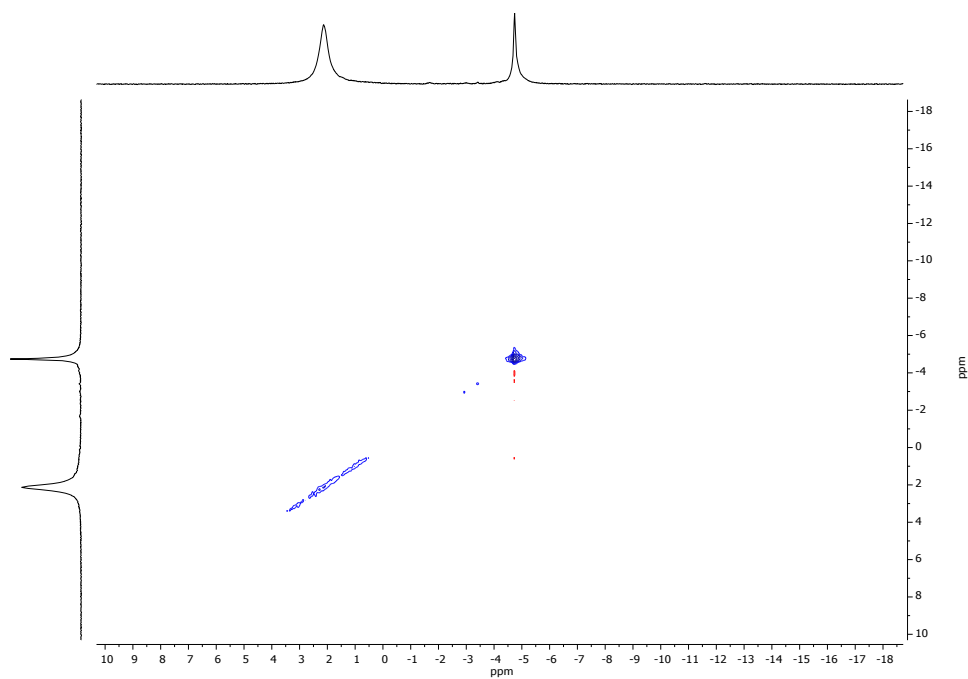


Figure S7k ${}^7\text{Li}$, ${}^7\text{Li}$ -NOESY spectrum of 7 (194 MHz, 263 K, C_7D_8).

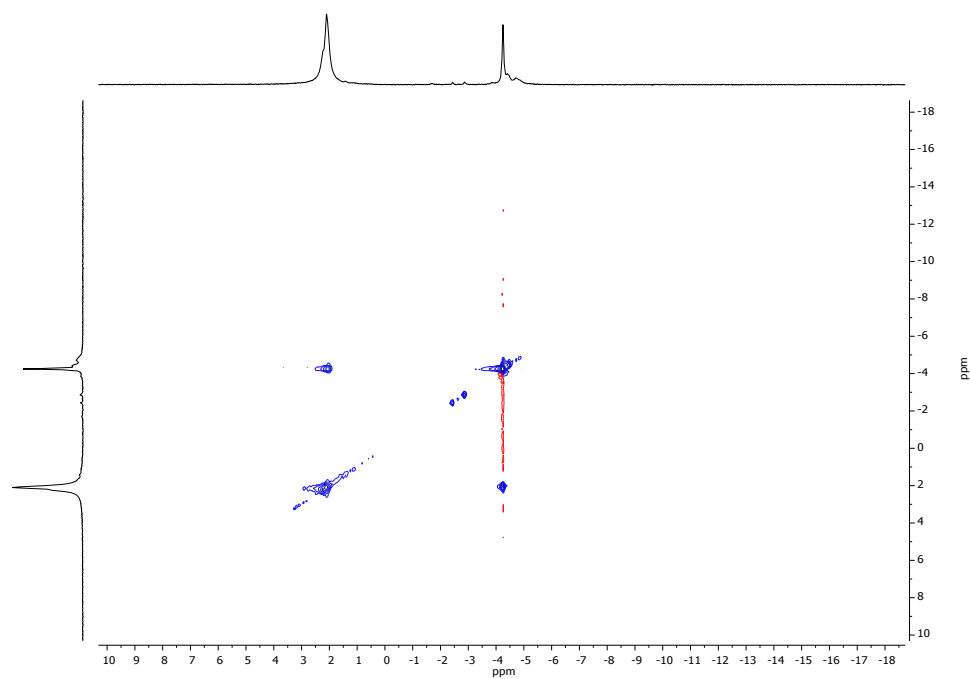


Figure S7l ^7Li , ^7Li -NOESY spectrum of **7** (194 MHz, 298 K, C_7D_8).

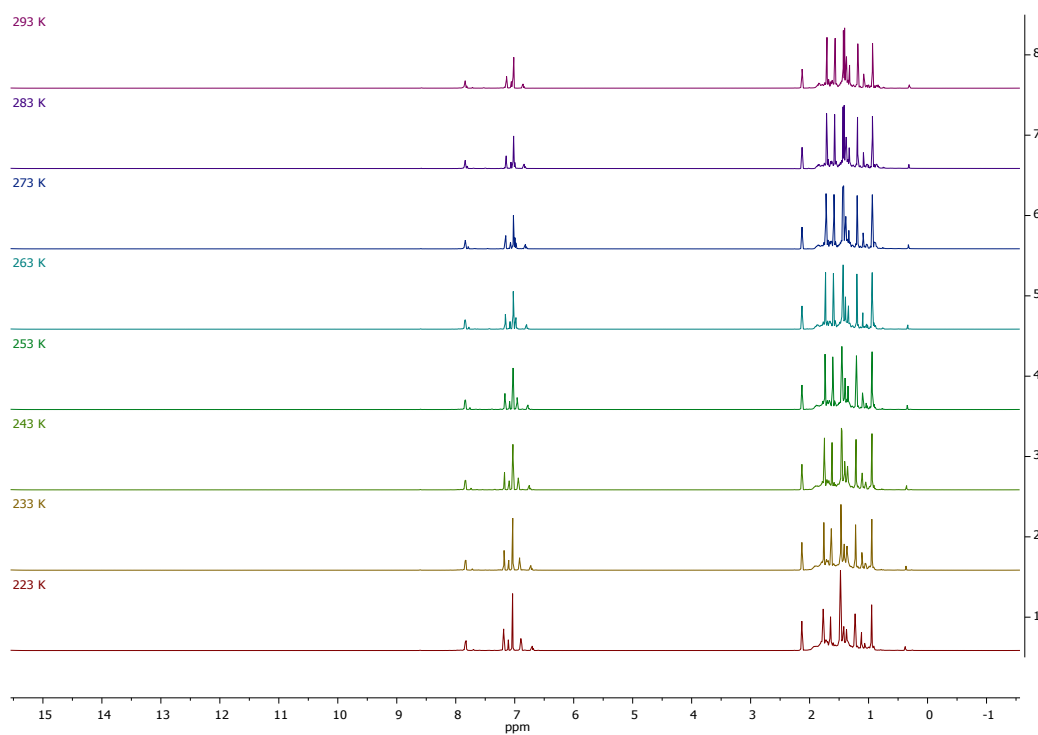


Figure S7m Variable temperature ^1H NMR spectra of **7** (500 MHz, T (specified), C_7D_8).

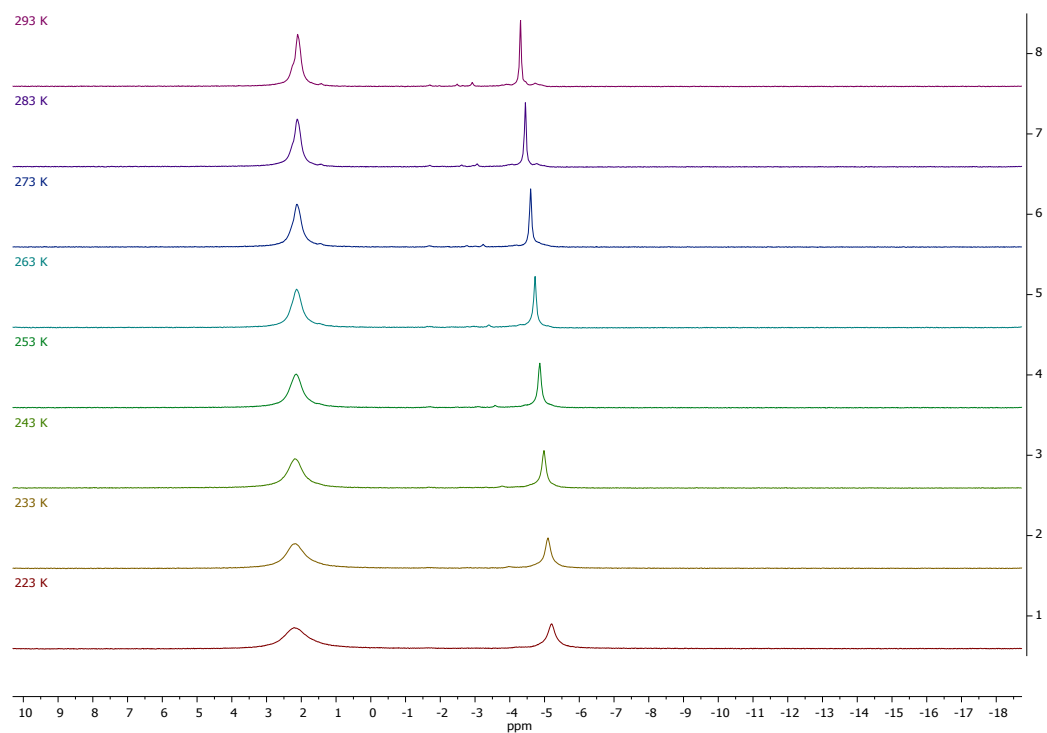


Figure S7n Variable temperature ^7Li NMR spectra of **7** (194 MHz, T (specified), C_7D_8).

DFT calculations

Computational Details

All calculations were carried with the Gaussian 16 program package.² The molecular structures and harmonic vibrational frequencies were obtained using the hybrid density functional method based on M06 functional.³ We used Ahlrichs' SVP⁴ all-electron basis set for Cu atom and 6-31+G* for the other atoms. Geometry optimization and vibrational analysis were performed at the same level. All the optimizations were calculated without any symmetry assumptions, and characterized by normal coordinate analysis at the same level of theory (number of imaginary frequencies, NIMAG, 0 for minima).

² Gaussian 16, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

³ (a) Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215-241; (b) Y. Zhao, D. G. Truhlar, *Acc. Chem. Res.*, 2008, **41**, 157-167.

⁴ A. Schäfer, H. Horn, R. Ahlrichs, *J. Chem. Phys.*, 1992, **97**, 2571-2577.

Structure optimisation for 1

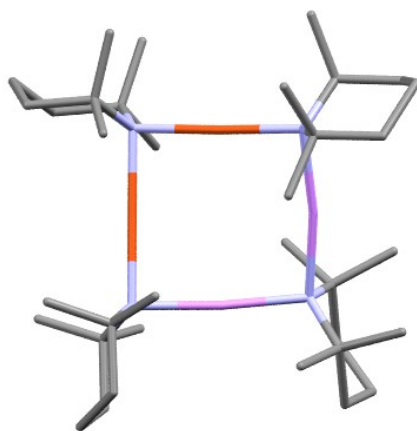


Figure S8 Optimised DFT molecular structure of **1**. $\Delta G = -3092241.394$
($\Delta E = -3092843.02$) kcal.mol⁻¹.

Structure optimisation for 2

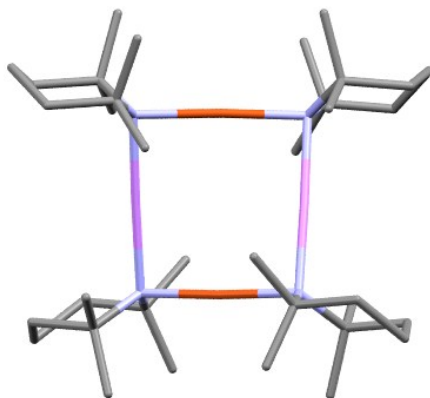
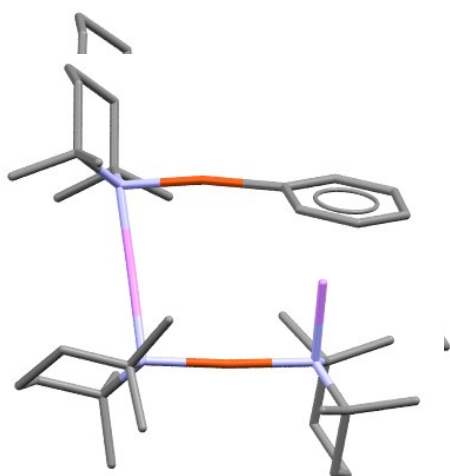


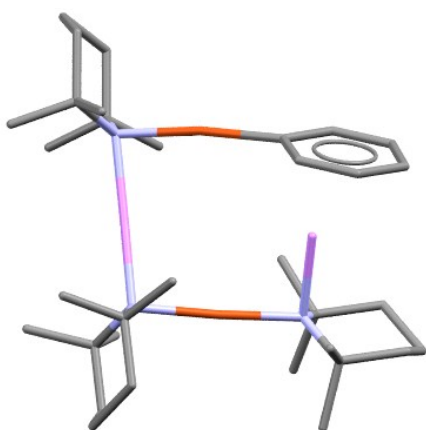
Figure S9 Optimised DFT structure of **2**. $\Delta G = -3092243.858$
($\Delta E = -3092845.838$) kcal.mol⁻¹.

Structure optimisation for 3

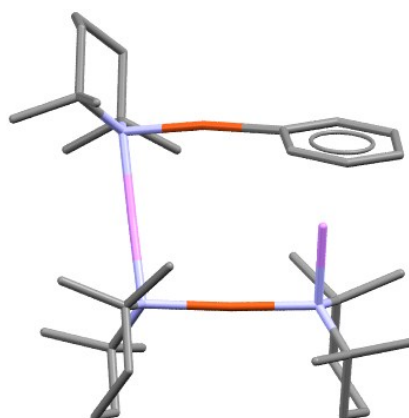


a) $\Delta G = -2981404.318$
($\Delta E = -2981901.61$) kcal.mol⁻¹

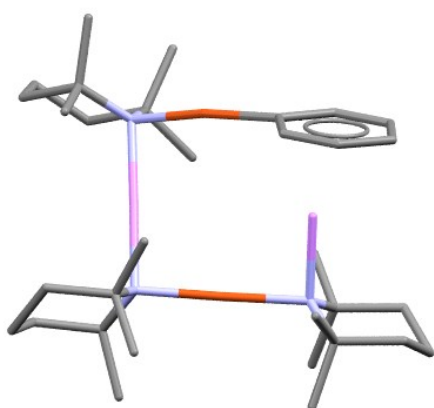
b) $\Delta G = -2981401.793$
($\Delta E = -2981898.945$) kcal.mol⁻¹



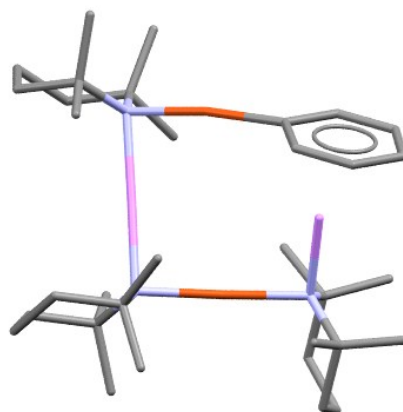
c) $\Delta G = -2981402.107$
($\Delta E = -2981898.932$) kcal.mol⁻¹



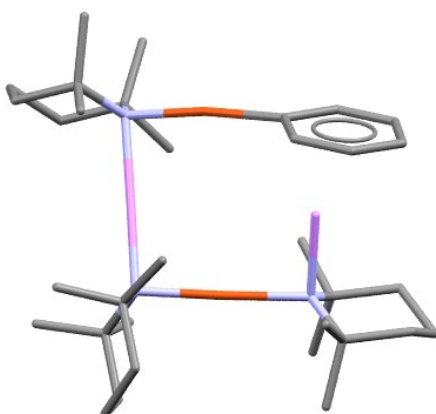
d) $\Delta G = -2981399.815$
($\Delta E = -2981896.846$) kcal.mol⁻¹



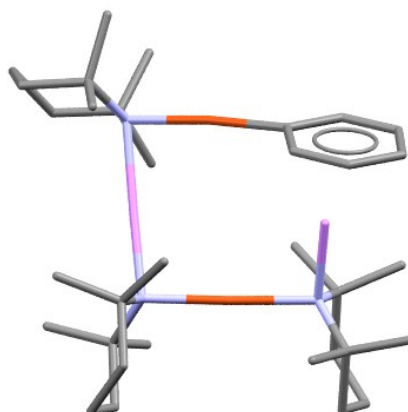
e) $\Delta G = -2981405.177$ (ΔE
 $= -2981901.73$) kcal.mol⁻¹



f) $\Delta G = -2981401.234$
 $(\Delta E = -2981898.267)$ kcal.mol⁻¹



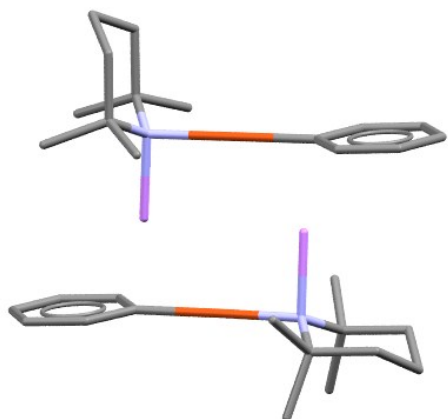
g) $\Delta G = -2981402.123$
 $(\Delta E = -2981899.13)$ kcal.mol⁻¹



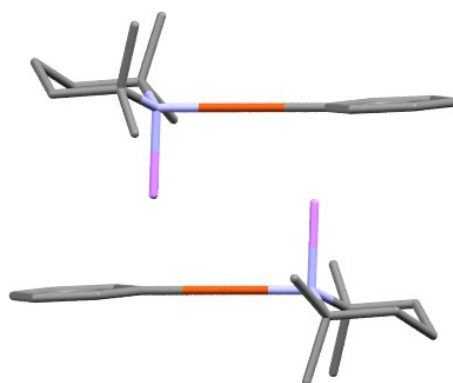
h) $\Delta G = -2981399.696$ (ΔE
 $= -2981897.131)$ kcal.mol⁻¹

Figure S10 Optimised DFT molecular structures for compound **3**.

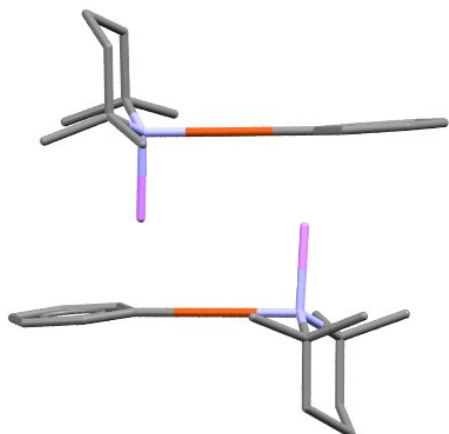
Structure optimisation for 4



a) $\Delta G = -2870563.837$
($\Delta E = -2870955.133$) kcal.mol⁻¹



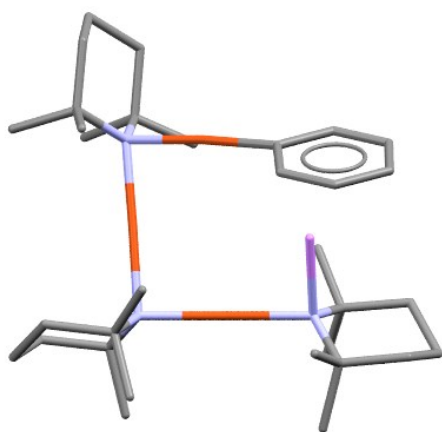
b) $\Delta G = -2870562.799$
($\Delta E = -2870952.95$) kcal.mol⁻¹



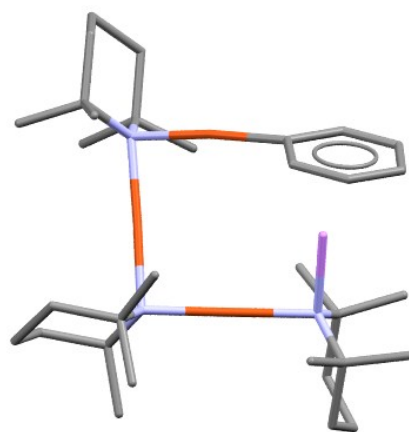
c) $\Delta G = -2870559.828$
($\Delta E = -2870951.038$) kcal.mol⁻¹

Figure S11 Optimised DFT molecular structures for **4**.

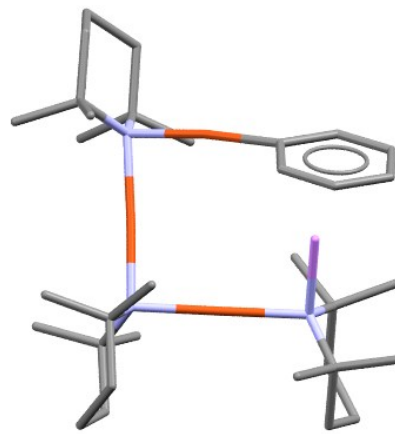
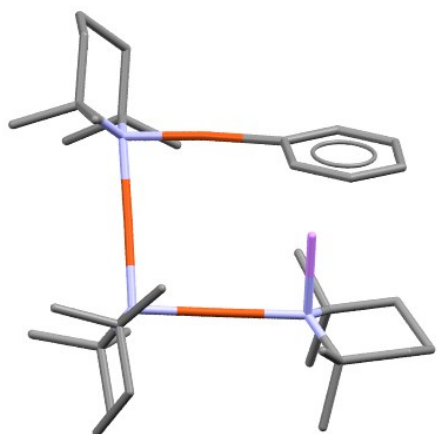
Structure optimisation for 5



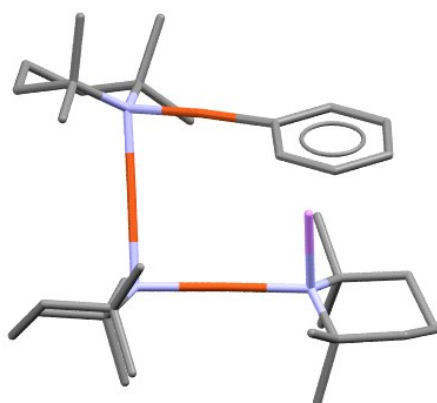
a) $\Delta G = -4005959.452$
($\Delta E = -4006456.917$) kcal.mol⁻¹



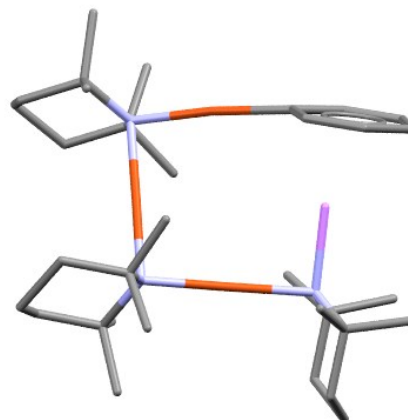
b) $\Delta G = -4005956.506$
($\Delta E = -4006454.084$) kcal.mol⁻¹



c) $\Delta G = -4005960.181$
($\Delta E = -4006456.712$) kcal.mol⁻¹

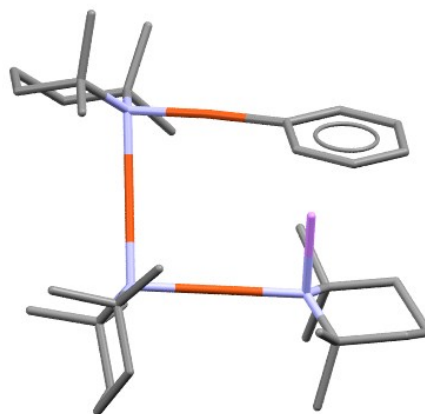


d) $\Delta G = -4005956.953$
($\Delta E = -4006454.234$) kcal.mol⁻¹



e) $\Delta G = -4005957.071$
($\Delta E = -4006455.214$) kcal.mol⁻¹

f) $\Delta G = -4005953.908$ (ΔE
 $= -4006451.922$) kcal.mol⁻¹



g) $\Delta G = -4005957.471$
 $(\Delta E = -4006455.071) \text{ kcal.mol}^{-1}$

h) $\Delta G = -4005954.173$
 $(\Delta E = -4006452.146) \text{ kcal.mol}^{-1}$

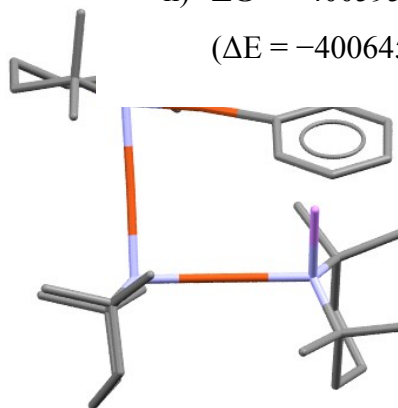
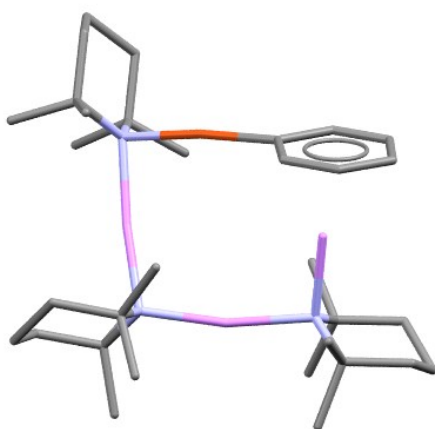
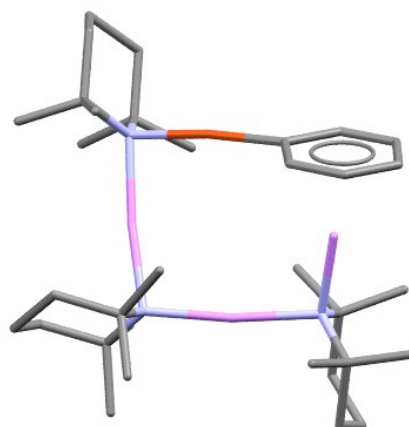


Figure S12 Optimised DFT structures for **5**.

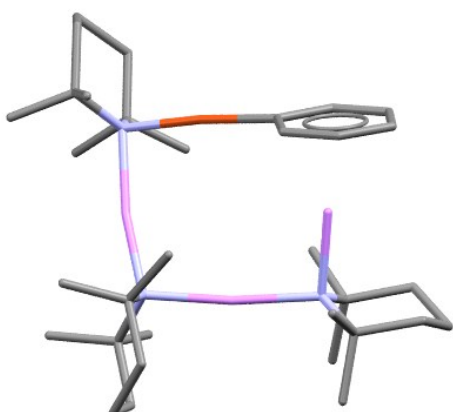
Structure optimisation for 7



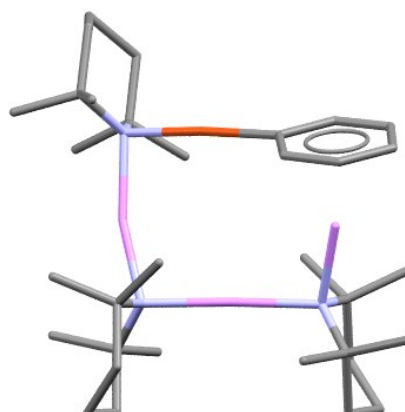
a) $\Delta G = -1956844.943$
($\Delta E = -1957341.434$) kcal.mol⁻¹



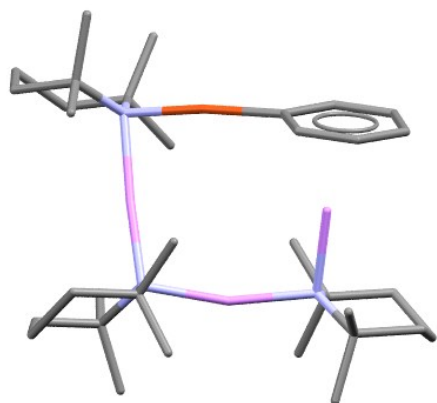
b) $\Delta G = -1956844.752$
($\Delta E = -1957341.321$) kcal.mol⁻¹



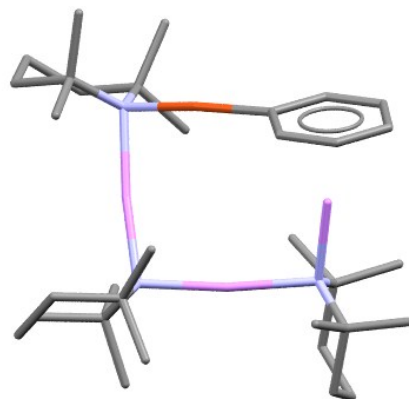
c) $\Delta G = -1956845.05$
($\Delta E = -1957341.157$) kcal.mol⁻¹



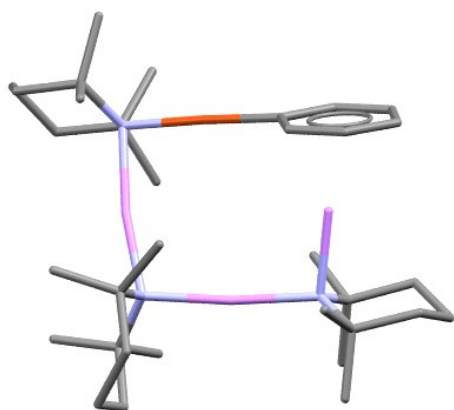
d) $\Delta G = -1956846.453$
($\Delta E = -1957341.731$) kcal.mol⁻¹



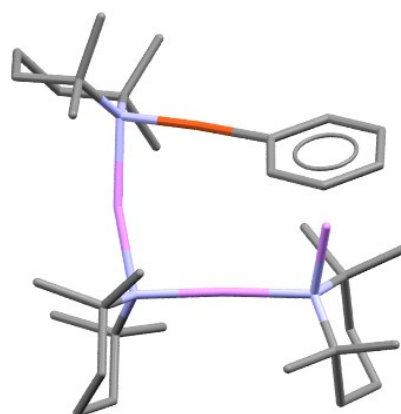
e) $\Delta G = -1956845.618$
 $(\Delta E = -1957341.988) \text{ kcal.mol}^{-1}$



f) $\Delta G = -1956844.613$
 $(\Delta E = -1957341.015) \text{ kcal.mol}^{-1}$



g) $\Delta G = -1956844.796$
 $(\Delta E = -1957340.762) \text{ kcal.mol}^{-1}$



h) $\Delta G = -1956844.493$
 $(\Delta E = -1957342.161) \text{ kcal.mol}^{-1}$

Figure S13 Optimised DFT molecular structures for **7**.

Structure optimization for 1

Cartesian Coordinates

Cu	1.15735600	-1.40851300	-0.01417400	C	5.12954100	0.11377500	0.09964300
Cu	-1.54245500	-0.92731000	0.04196600	H	4.91638200	1.14036000	0.45007200
N	2.74640700	-0.37312900	-0.44572900	H	5.98863100	-0.24488000	0.68999200
N	-0.39905200	-2.49677700	0.43749400	C	-0.46260000	-1.64282500	2.74200600
C	3.01830300	-0.26236200	-1.90401300	H	-1.26222100	-0.94879500	2.44984200
N	-2.65729000	0.61709200	-0.42059100	H	0.49486800	-1.10930800	2.66241900
C	3.90414500	-0.76637300	0.40151000	H	-0.61481900	-1.90227500	3.79938400
N	0.55465700	2.84413200	0.39641300	C	-4.54154500	2.16906300	0.12013000
C	-0.62224500	-3.61146700	-0.54063300	H	-5.35424700	2.34122800	0.84462400
C	-0.47724800	-2.89920200	1.87963800	H	-3.88989900	3.06177300	0.16462200
C	-3.71468600	0.94982500	0.57186500	C	3.18135900	-1.60033000	-2.64912800
C	-1.93364700	-4.34815100	-0.22348100	H	2.35935300	-2.28614500	-2.39874800
H	-2.04800500	-5.19817100	-0.91604800	H	4.11922400	-2.11574900	-2.41857200
H	-2.77305800	-3.65906800	-0.42642900	H	3.16432500	-1.43806800	-3.73777400
C	-1.79270200	-3.64298200	2.15891200	C	-2.02726400	-4.81442200	1.21958600
H	-2.62508300	-2.92483900	2.05095900	H	-1.29634500	-5.61595000	1.41334100
H	-1.80008000	-3.97937800	3.20879800	H	-3.01477900	-5.25959500	1.40942400
C	1.82182000	0.43807800	-2.54755000	C	-4.65279800	-0.21966800	0.91791600
H	1.67313400	1.45812300	-2.15295000	H	-4.06405900	-1.10172600	1.21526500
H	0.89222700	-0.12842700	-2.38864000	H	-5.29359500	-0.52067400	0.08267000
H	1.96405500	0.55128500	-3.63174400	H	-5.31356100	0.04440200	1.75809300
C	-3.11534300	0.53183200	-1.83605600	C	0.63223300	1.76167200	2.55648900
C	4.25470000	0.61613000	-2.16391700	H	-0.45505200	1.61064700	2.58799300
H	4.46704000	0.63794700	-3.24546700	H	0.99560000	1.78584200	3.59475000
H	4.01369200	1.65578200	-1.87224800	H	1.06800200	0.86447800	2.08780400
C	-0.75710000	-3.02714500	-1.94317300	C	0.98809600	3.03976000	1.79655700
H	-1.61458800	-2.34721200	-2.01568700	C	4.30805300	-2.25000400	0.29694100
H	-0.91441200	-3.83074600	-2.67656500	H	4.80714000	-2.50344600	-0.64433900
H	0.14647600	-2.47436100	-2.24302600	H	3.42236900	-2.89643800	0.38592500
C	0.52281900	4.06659500	-0.43060900	H	5.00238100	-2.51627800	1.10845900

C 5.47539800 0.16982600 -1.37835600
H 6.31161800 0.86373100 -1.54817400
H 5.82440700 -0.81342200 -1.73254500
C -0.19593300 5.23008700 0.27959800
H -1.26924800 4.97284900 0.35300600
H -0.13261300 6.14090400 -0.33924300
C -3.04601600 1.36654400 1.88079000
H -2.39020000 2.24424700 1.74705900
H -2.45413900 0.55188500 2.31926200
H -3.80062100 1.65857200 2.62512400
C 0.32703100 5.49162100 1.68146200
H 1.35931000 5.87637200 1.64239300
H -0.26583900 6.27948100 2.16916300
C 0.70758900 -3.75070500 2.37515100
H 0.65323500 -4.80397100 2.08370100
H 0.74066300 -3.73202300 3.47440400
H 1.66153600 -3.34931000 2.00584500
C -3.93691600 1.76927900 -2.23941800
H -3.26826300 2.64834500 -2.25605700
H -4.30195700 1.63553600 -3.27109700
C 3.53312900 -0.53073600 1.86484400
H 3.26254600 0.51786900 2.05296400
H 4.38242100 -0.76903400 2.52141900
H 2.68820200 -1.16377700 2.17664600
C -3.94545500 -0.72359000 -2.18409100
H -3.53670800 -1.62051600 -1.69940600
H -3.94260100 -0.89565000 -3.27139600
H -4.99593800 -0.64422500 -1.88138600

C -1.87805000 0.51080200 -2.73183100
H -1.24249400 1.38976900 -2.55697100
H -2.16537300 0.52273700 -3.79341400
H -1.26656900 -0.38563900 -2.56576400
C 1.90584200 4.53968200 -0.92541200
H 2.55321900 4.90552900 -0.12149900
H 1.80704700 5.35641800 -1.65763700
H 2.43562000 3.71288900 -1.42613000
C -5.08685400 2.04963700 -1.28967400
H -5.84462500 1.25187400 -1.34562000
H -5.60483900 2.97630300 -1.57753200
C 2.51275100 3.26143700 1.97963100
H 3.11673100 2.58658900 1.34942900
H 2.81363700 3.08017100 3.02307300
H 2.83006000 4.28001500 1.73028300
C -0.28351400 3.76562600 -1.69416400
H -1.32581800 3.48581600 -1.45958100
H 0.17393000 2.95509600 -2.28125000
H -0.34441000 4.64787300 -2.34767500
C 0.26126100 4.20596900 2.48939200
H -0.79933800 3.92619500 2.61923900
H 0.67441100 4.35412800 3.50165600
C 0.53960100 -4.61829600 -0.62303400
H 1.50039400 -4.09358100 -0.72859200
H 0.41088100 -5.26139400 -1.50589400
H 0.61760700 -5.28334100 0.24126000
Li -1.08089200 1.80960500 -0.01748000
Li 1.78266600 1.32709200 -0.01234600

Structure optimization for 2

Cartesian Coordinates

C	3.85513200	-1.98789400	2.25497500	C	-2.43483400	-2.73040600	0.42011400
C	2.37050000	-2.10600700	1.86908600	C	-3.92833800	-2.65016100	0.06592200
C	3.04833600	-2.37081700	-0.53972800	C	-4.21712200	-2.93878900	-1.39758100
C	4.52220600	-2.24508200	-0.11394300	H	-3.70548700	-0.99334300	-2.14191900
C	4.77842100	-2.72655400	1.30257900	H	-3.52671900	-2.27751000	-3.34474000
H	4.13248300	-0.91854700	2.25714200	H	-4.48937700	-3.34167100	0.71609400
H	3.98942800	-2.34637800	3.28870900	H	-4.28281500	-1.63146400	0.30608000
H	5.15610000	-2.78670700	-0.83526800	H	-4.01938800	-3.99794300	-1.62816500
H	4.81201400	-1.17951700	-0.17923400	H	-5.28482800	-2.78254500	-1.60989400
H	4.62156700	-3.81474900	1.37604900	N	-1.62869900	-1.86378500	-0.50211300
H	5.82922900	-2.55549000	1.57886800	C	-1.30042100	-3.44480800	-2.48304200
N	2.15135100	-1.71567500	0.44951300	H	-1.30524400	-3.44093900	-3.58301300
C	1.86770400	-3.51387100	2.24503300	H	-0.25905700	-3.57633300	-2.15575800
H	1.86942400	-3.63894100	3.33883900	H	-1.86269200	-4.32840700	-2.16918200
H	0.83629900	-3.66370900	1.89350900	C	-1.16380900	-1.03234400	-2.77311200
H	2.47668600	-4.32408400	1.83101400	H	-0.07238100	-1.09349800	-2.65674000
C	1.59616600	-1.13530600	2.75550600	H	-1.39174500	-1.14816600	-3.84251700
H	0.51282500	-1.22277300	2.59547200	H	-1.47693800	-0.02553900	-2.47310300
H	1.79195800	-1.33711100	3.81876600	C	-1.98709500	-4.20520100	0.45574200
H	1.88359900	-0.09301100	2.56287200	H	-0.89012100	-4.28100500	0.46594400
C	2.72592300	-3.84778400	-0.83752900	H	-2.36597200	-4.68788300	1.36837600
H	1.64832000	-3.97649400	-1.01892800	H	-2.35346500	-4.80133300	-0.38569800
H	3.26358000	-4.18696500	-1.73625300	C	-2.28494400	-2.21893100	1.84935800
H	3.00443300	-4.52718100	-0.02512600	H	-2.91216000	-2.81136800	2.53051100
C	2.91245200	-1.62952900	-1.86809100	H	-1.24670900	-2.29749600	2.20405200
H	3.58505000	-2.05593200	-2.62584700	H	-2.60506500	-1.17127100	1.93611600
H	1.88712600	-1.69238500	-2.26369000	C	-3.32425100	1.82535100	2.51070500
H	3.18947500	-0.56550600	-1.77387000	C	-1.94527100	2.18359700	1.93443300
C	-3.37128400	-2.03646800	-2.28033400	C	-2.98630900	2.63779600	-0.29861300
C	-1.86936900	-2.11234200	-1.96160500	C	-4.36393500	2.27504200	0.28200900

C -4.46255000 2.52303800 1.78003000
H -3.46510900 0.73368900 2.42521400
H -3.35092900 2.06320500 3.58767500
H -5.15147700 2.83155000 -0.25358900
H -4.54373900 1.20239600 0.08501500
H -4.44539000 3.60505700 1.98917400
H -5.43025000 2.16392200 2.15993500
N -1.89133800 1.96931300 0.45902500
C -1.56643600 3.61280400 2.38386200
H -1.28960800 3.60981300 3.44835700
H -0.69810000 3.99302300 1.82162800
H -2.37052600 4.34617000 2.27268100
C -0.89808400 1.28047100 2.57890400
H 0.12332200 1.55939600 2.26607400
H -0.92582100 1.35872300 3.67557300
H -1.04736600 0.22755300 2.31269000
C -2.84992600 4.17205200 -0.38113700
H -1.82615100 4.45980700 -0.66459000
H -3.52695500 4.56798800 -1.15216600
H -3.09462300 4.69571300 0.54715500
C -2.95315000 2.15885100 -1.74719000
H -3.74347300 2.64931300 -2.33335800
H -1.99038600 2.39241900 -2.22933600
H -3.12175600 1.07533100 -1.81670300
C 3.24839200 2.75026100 -2.48796200
C 1.86636000 2.65136200 -1.81997300
C 2.93097700 2.93668400 0.42199600
C 4.30651800 3.03588500 -0.26409400

C 4.22619700 3.58580400 -1.67825500
H 3.65746400 1.72892500 -2.58865300
H 3.14211400 3.14903400 -3.51102500
H 4.99037800 3.64129300 0.35433100
H 4.73969300 2.01915300 -0.31089500
H 3.91404900 4.64306100 -1.66423400
H 5.22011200 3.57434900 -2.14948900
N 1.94693600 2.21393100 -0.40841700
C 1.12041700 3.98959900 -2.04595900
H 0.90069500 4.13750100 -3.11452200
H 0.14988800 4.01337500 -1.51975500
H 1.68303200 4.86660800 -1.70988600
C 1.06093000 1.59642500 -2.57403800
H 0.05659800 1.46146300 -2.13998400
H 0.91789000 1.86835100 -3.63050300
H 1.56026400 0.61874400 -2.54871500
C 2.48468700 4.34251800 0.87618000
H 1.48254800 4.29632900 1.33282000
H 3.17116400 4.74881700 1.63538000
H 2.44274300 5.07269100 0.06129300
C 3.13385800 2.13997200 1.70971600
H 3.86156200 2.62909400 2.37318900
H 2.19155400 2.04396700 2.27206000
H 3.53138100 1.12941900 1.51042900
Li 2.10712200 0.27189600 0.01500400
Cu 0.26639700 -1.78634200 -0.03259000
Cu -1.76464000 0.05662700 -0.01353100
Li 0.01247800 2.30805900 0.00996900

Structure optimization for 3

3-a)

Cartesian Coordinates

C	-4.13088600	-0.52598900	-0.60288600	C	5.47978500	-1.12202500	1.28980500
C	-3.26798600	-0.92743500	1.72606100	C	4.20019600	-1.52826400	2.00208100
C	-4.14773300	-2.18433900	1.82724400	H	4.86609800	-1.78620400	-0.65503500
C	-5.39301800	-2.10124400	0.95780000	H	6.08987600	-0.50979000	-0.70234600
C	-5.00940200	-1.78242900	-0.47900200	H	6.23419200	-1.91756800	1.37839600
H	-3.54470300	-3.05091400	1.50179000	H	5.92242800	-0.23418900	1.76930200
H	-4.42053400	-2.36352100	2.88111400	H	3.85206400	-2.49030500	1.58163700
H	-5.94731700	-3.05041600	0.99939000	H	4.38676700	-1.70523300	3.07407900
H	-6.08382500	-1.33619400	1.34867800	N	2.86015800	-0.16502800	0.41172500
H	-4.44246700	-2.63536300	-0.89320500	Cu	1.36878500	1.03765000	0.11456100
H	-5.91108100	-1.66688300	-1.10383800	Li	1.85675000	-1.57867500	-0.48345200
N	-2.96035600	-0.59003300	0.31100900	C	2.39459900	-3.93721500	-1.94970100
Cu	-1.57520500	-1.76803400	-0.39667300	C	1.85736300	-4.25845400	-0.70181300
C	-0.23830600	2.56130200	-1.68330300	C	0.65670900	-3.67339200	-0.28461600
C	-0.36060000	3.24410000	0.74267400	C	-0.06102700	-2.74216400	-1.07092500
C	-1.67228200	3.99389800	0.44676600	C	0.50959100	-2.46649900	-2.33520800
C	-1.77730800	4.47055400	-0.99316700	C	1.70464300	-3.04641000	-2.77381700
C	-1.55921100	3.30580600	-1.94676200	H	3.33764000	-4.37491900	-2.27527700
H	-2.51958500	3.31158000	0.65329200	H	2.38115400	-4.95668600	-0.04751600
H	-1.78200000	4.83815800	1.14703400	H	0.27587500	-3.94323200	0.70430400
H	-2.76280300	4.92596700	-1.16979500	H	0.01414700	-1.75351800	-3.00064000
H	-1.04040100	5.26657100	-1.18626700	H	2.10896800	-2.78841800	-3.75367300
H	-2.39790700	2.59254600	-1.83398200	C	3.68860600	0.17721000	-1.85596900
H	-1.58691500	3.64888500	-2.99415200	H	3.27404400	-0.79781000	-2.16436500
N	-0.14544700	2.16975400	-0.25562500	H	2.94988100	0.95570200	-2.09782600
C	3.07356800	-0.49311300	1.84344200	H	4.57330800	0.35508600	-2.48452000
C	4.06617500	0.19968000	-0.37353500	C	4.61924900	1.60896700	-0.09428600
C	5.18135200	-0.84155200	-0.17331700	H	5.11103600	1.69716900	0.88042500

H	5.36277400	1.88943300	-0.85623300	C	-0.23731900	1.27903700	-2.52049600
H	3.80720200	2.35089100	-0.12427500	H	0.75431800	0.80159100	-2.52215400
C	3.36295100	0.71646700	2.75155700	H	-0.95532400	0.53120900	-2.14791300
H	3.27930400	0.43033000	3.81127600	H	-0.50416700	1.49598000	-3.56589200
H	4.36536400	1.13539800	2.61225000	C	-3.62593100	-0.45860800	-2.04512500
H	2.64005800	1.52337200	2.56098500	H	-3.08226000	0.47907700	-2.23782700
C	1.78670400	-1.12707800	2.37085900	H	-2.95531900	-1.29952400	-2.28728600
H	0.94576300	-0.41850100	2.32640700	H	-4.47019400	-0.49312400	-2.74918400
H	1.50096400	-2.02465900	1.79723300	C	-4.99606900	0.73588000	-0.41695700
H	1.90372100	-1.44230500	3.41789900	H	-4.36193800	1.63540600	-0.37018000
C	0.79694400	4.24891200	0.88016800	H	-5.68119200	0.85598800	-1.26962900
H	0.90061700	4.91411200	0.01640800	H	-5.61464900	0.72057500	0.48606200
H	0.64981800	4.88808400	1.76433600	C	-3.92734700	0.22143200	2.51596100
H	1.75071000	3.71399100	1.00425100	H	-4.98550500	0.36836000	2.27753300
C	-0.51211900	2.58235000	2.11274900	H	-3.87149100	0.02210800	3.59653100
H	0.40707500	2.05410600	2.40956900	H	-3.41394200	1.17617300	2.32629600
H	-0.73430500	3.33010400	2.88771900	C	-1.95080300	-1.22233700	2.44564300
H	-1.34106700	1.85548200	2.13399900	H	-1.41034100	-2.06194200	1.97978200
C	0.93059000	3.41255100	-2.21710600	H	-1.28047800	-0.34734300	2.44001800
H	0.92940900	3.41190600	-3.31815200	H	-2.13143900	-1.48432900	3.49842100
H	0.89037800	4.46056300	-1.90057400	Li	-1.54657000	0.79712800	0.10586800
H	1.89327800	3.00231900	-1.87934300				

3-b)

Cartesian Coordinates

C	-4.13431000	-0.35482200	-0.58531900	H	-3.79136700	-2.81711300	1.63523800
C	-3.29138600	-0.72716600	1.75873000	H	-4.57166300	-1.97982900	2.98875500
C	-4.29644600	-1.87847300	1.92527800	H	-6.18933100	-2.58672000	1.15744200
C	-5.53679400	-1.70635200	1.06258600	H	-6.13639500	-0.85149000	1.41631000
C	-5.13417700	-1.50711400	-0.38996400	H	-4.65933300	-2.43470000	-0.75655700

H	-6.02341200	-1.33490600	-1.01951900	C	0.36728600	-2.59507600	-2.27227200
N	-2.96853500	-0.48302200	0.32826200	C	1.54703600	-3.21182900	-2.70336700
Cu	-1.66614600	-1.76596100	-0.34103400	H	3.14709000	-4.57328700	-2.18295100
C	-0.13724100	2.47336200	-1.75469100	H	2.18947300	-5.07801600	0.06243600
C	-0.16013600	3.22370300	0.64535000	H	0.12617400	-3.97969600	0.81073500
C	-1.48746900	3.96192200	0.38712000	H	-0.11530000	-1.88791200	-2.95286800
C	-1.67190400	4.38626100	-1.06140500	H	1.95283500	-2.98603500	-3.69042400
C	-1.47471400	3.19822000	-1.99079600	C	1.64371900	-0.84234500	2.41591000
H	-2.32103200	3.28848100	0.66661100	H	1.02744300	0.05279100	2.25209900
H	-1.56312000	4.83266000	1.05898600	H	1.10514100	-1.70182300	1.98195200
H	-2.67495600	4.81532400	-1.20372100	H	1.70972200	-1.00833700	3.50116500
H	-0.96385100	5.19157700	-1.31438500	C	3.76834000	-2.00224600	2.14023700
H	-2.30200900	2.48085200	-1.83184700	H	3.61108600	-2.25479700	3.19923100
H	-1.54326900	3.51387500	-3.04514600	H	3.37646500	-2.83872300	1.54047000
N	0.00201800	2.11310100	-0.32236500	H	4.85058200	-1.96195100	1.98599500
C	4.10603100	-0.07012700	-0.38937100	C	5.09925000	-1.23513700	-0.58158200
C	3.03352800	-0.68914400	1.79956600	H	5.84195400	-0.97186900	-1.34914400
C	3.74820200	0.49065000	2.47797700	H	5.66090600	-1.49743400	0.31984400
C	5.04838100	0.87010100	1.78064400	H	4.57814100	-2.14316800	-0.92459700
C	4.81742900	1.10820900	0.29383800	C	3.71428100	0.35479800	-1.80402900
H	3.06853500	1.36165000	2.46008200	H	3.22383500	-0.46956300	-2.35063100
H	3.93419700	0.25625100	3.53981800	H	3.02490400	1.21041700	-1.79376700
H	5.47405000	1.77206200	2.24428700	H	4.60123100	0.64839100	-2.38374600
H	5.80233600	0.07906700	1.92566800	C	1.00249800	4.23131200	0.68657600
H	4.18746600	2.00753300	0.16769500	H	0.90668600	4.89144900	1.56241400
H	5.77332400	1.31683000	-0.21584900	H	1.96065900	3.69627600	0.76883100
N	2.86526700	-0.44136500	0.34210700	H	1.05605100	4.87542300	-0.19700200
Cu	1.45385200	0.88854800	0.03396000	C	-0.23984500	2.62730500	2.05065100
Li	1.84150500	-1.81448500	-0.54533000	H	0.72287200	2.19475900	2.35969200
C	2.21785300	-4.10350900	-1.86267300	H	-0.50712000	3.40077600	2.78539300
C	1.67933000	-4.38203900	-0.60480400	H	-1.00596400	1.83810200	2.13015900
C	0.50018200	-3.75102000	-0.19097200	C	0.99864400	3.33335300	-2.34727800
C	-0.19998600	-2.82223800	-0.99606700	H	1.01249100	3.23984500	-3.44407900

H	0.89838200	4.40159100	-2.12468800	H	-5.47372600	1.09039800	0.44140700
H	1.97647100	3.00832300	-1.96629800	H	-4.15213200	1.83110100	-0.47631900
C	-0.14834000	1.17245700	-2.56246800	C	-3.81515900	0.51903300	2.50049800
H	0.85290500	0.71784200	-2.60196300	H	-4.84587800	0.78232500	2.24250100
H	-0.83082600	0.41878200	-2.13674900	H	-3.79232900	0.35442000	3.58813800
H	-0.47081400	1.35960100	-3.59805700	H	-3.18944900	1.39882800	2.28495200
C	-3.63763600	-0.42340900	-2.03083300	C	-2.00470800	-1.13198400	2.48002100
H	-2.98945600	0.43079800	-2.27836900	H	-1.57539900	-2.05353200	2.05529400
H	-3.07218700	-1.34928200	-2.22659800	H	-1.23424800	-0.34604500	2.41898200
H	-4.48689600	-0.39868300	-2.72940700	H	-2.19717200	-1.31430200	3.54748800
C	-4.86950200	0.99487000	-0.46658300	Li	-1.46524700	0.80850700	0.08516500
H	-5.55170000	1.13354900	-1.31881700				

3-c)

Cartesian Coordinates

C	-4.15773700	-0.34530500	-0.68452800	C	0.97239500	3.62640000	-1.92125500
C	-3.39556800	-0.72702500	1.68766100	C	0.93754500	4.78854600	-0.93554600
C	-4.41655400	-1.86857600	1.81772500	C	0.89995100	4.28742300	0.50317100
C	-5.62331900	-1.68605600	0.90982400	H	1.93802300	3.09999600	-1.81648100
C	-5.16849600	-1.49311700	-0.52898300	H	0.92703200	4.00078800	-2.95813700
H	-3.90906100	-2.81104000	1.54496500	H	1.81564200	5.43370600	-1.08536900
H	-4.73168600	-1.96875500	2.87010100	H	0.06326100	5.42953800	-1.13555200
H	-6.28703000	-2.56009500	0.98290300	H	1.86099200	3.79416400	0.73734400
H	-6.22663200	-0.82496000	1.24157400	H	0.80122100	5.13503000	1.20235600
H	-4.68446400	-2.42342200	-0.87577700	N	-0.18260400	2.17561600	-0.25753600
H	-6.03377400	-1.31792800	-1.19036300	C	2.93069500	-0.65412000	1.85874000
N	-3.02897400	-0.48258800	0.27043500	C	4.01591500	-0.04162800	-0.32944600
Cu	-1.68934300	-1.73957500	-0.37155500	C	4.98409300	-1.22703400	-0.15797800
C	-0.22654300	3.27065100	0.74722800	C	5.22756200	-1.60056400	1.29485300
C	-0.15795400	2.61316300	-1.67901700	C	3.90098200	-1.84028300	1.99719800

H	4.55491200	-2.10314900	-0.68102500
H	5.93556400	-0.99896000	-0.66605600
H	5.85876200	-2.49938200	1.35519500
H	5.79296400	-0.80366800	1.80401800
H	3.42274100	-2.73745900	1.56004400
H	4.05908700	-2.06206800	3.06562400
N	2.76416300	-0.28383800	0.42998000
Cu	1.32757800	0.98245600	0.10544500
Li	1.71699000	-1.66228600	-0.47399500
C	2.19208600	-4.06282400	-1.92425100
C	1.65467800	-4.35915100	-0.67038800
C	0.47904300	-3.73068200	-0.24517400
C	-0.21496000	-2.78179000	-1.03164100
C	0.35357400	-2.53317200	-2.30293800
C	1.52610500	-3.15340200	-2.74758500
H	3.11722600	-4.53373400	-2.25484700
H	2.16027900	-5.07129400	-0.01672800
H	0.09969600	-3.97963100	0.74985800
H	-0.12410600	-1.80929300	-2.96965700
H	1.93080200	-2.91392100	-3.73195500
C	3.67342900	0.04522700	-1.81761500
H	3.08827900	-0.82204500	-2.16887100
H	3.10485300	0.95697900	-2.04897800
H	4.59246400	0.07005100	-2.42116000
C	4.73642700	1.27519800	0.01017700
H	5.22279300	1.26668600	0.99113400
H	5.51799600	1.48839200	-0.73530400
H	4.02088800	2.11101000	-0.00037600
C	3.39725400	0.48471100	2.78729700
H	3.18523600	0.23210400	3.83736600
H	4.47216200	0.68616600	2.72239200
H	2.87374000	1.42184400	2.55221000
C	1.56938000	-1.10767200	2.38578400

H	1.65687300	-1.49460000	3.41159800
H	0.85095300	-0.27484600	2.40437800
H	1.13156100	-1.91488400	1.77530500
C	-1.48926900	3.20580300	-2.18828200
H	-1.67287400	4.23435500	-1.86338700
H	-1.49798300	3.21822600	-3.28817200
H	-2.34775300	2.59830100	-1.86210600
C	0.08606500	1.37865800	-2.54909600
H	-0.72074200	0.63638400	-2.42559800
H	0.12521000	1.65120800	-3.61387000
H	1.03147300	0.87946400	-2.29613700
C	-1.58242900	4.00215200	0.82470200
H	-1.63405900	4.60182600	1.74539800
H	-1.76916200	4.68702500	-0.00732700
H	-2.41786500	3.28383100	0.85580700
C	-0.03183000	2.65092300	2.13061100
H	-0.83603300	1.93219900	2.36691800
H	0.92732600	2.11957300	2.20752200
H	-0.04755900	3.42397200	2.91231100
C	-3.59600100	-0.40691400	-2.10636400
H	-2.90771500	0.43086600	-2.30392600
H	-3.05065300	-1.34668500	-2.29070800
H	-4.40692800	-0.34122400	-2.84653700
C	-4.89332100	1.00637100	-0.58773200
H	-4.17525000	1.84065200	-0.54545600
H	-5.52818800	1.16010300	-1.47318000
H	-5.54646500	1.09137900	0.28703900
C	-3.91964300	0.52657900	2.41523700
H	-4.92003500	0.83563900	2.09671500
H	-3.97059300	0.34747600	3.49971300
H	-3.24391100	1.38230300	2.25347000
C	-2.13270200	-1.14113300	2.44353700
H	-1.69418000	-2.06343500	2.02979500

H -1.36131300 -0.35428000 2.39939800
H -2.35338800 -1.32137100 3.50591700

Li -1.58453200 0.84724600 0.06937700

3-d)

Cartesian Coordinates

C -4.21072800 -0.10523000 -0.58984000
C -3.37843700 -0.46248500 1.76084800
C -4.43666500 -1.55924800 1.95835100
C -5.66910000 -1.34811600 1.09229000
C -5.26284100 -1.20457700 -0.36657300
H -3.97717900 -2.52732600 1.69023800
H -4.71469400 -1.62213000 3.02398900
H -6.36368800 -2.19281600 1.20999200
H -6.22459400 -0.45670100 1.42728400
H -4.83411200 -2.16257200 -0.71082400
H -6.14537500 -1.00561200 -0.99780400
N -3.05169400 -0.26948400 0.32537400
Cu -1.82188900 -1.62288300 -0.34715700
C 0.16106100 3.28215300 0.65016600
C -0.07274800 2.48368000 -1.72122900
C 1.04364300 3.44723800 -2.15502900
C 1.15505800 4.66456000 -1.24699400
C 1.28501000 4.23265800 0.20666600
H 2.00304700 2.90312700 -2.13565900
H 0.87998500 3.75751100 -3.20103200
H 2.02357800 5.27286300 -1.53919200
H 0.27841500 5.32078700 -1.37301400
H 2.24656000 3.70309400 0.33545600
H 1.31535400 5.11277300 0.87094100
N 0.03202000 2.12890900 -0.27860900

C 4.04831500 -0.30895100 -0.29386200
C 2.83359900 -1.04238600 1.78406100
C 3.66912500 -0.05311900 2.61194400
C 5.02911800 0.23482100 1.99290200
C 4.86406600 0.68423700 0.54871500
H 3.10912300 0.89482100 2.68995300
H 3.78302000 -0.43548100 3.64029400
H 5.55057400 1.01033100 2.57291400
H 5.67310900 -0.65836700 2.04502500
H 4.33502800 1.65452900 0.53712700
H 5.84779100 0.85239700 0.07894900
N 2.74878200 -0.62963900 0.35459800
Cu 1.41582100 0.78370700 0.05857100
Li 1.66246600 -1.89899000 -0.62611800
C 1.84902400 -4.18465400 -2.03728200
C 1.31657900 -4.47433700 -0.77961000
C 0.19893000 -3.77352600 -0.31144900
C -0.44635000 -2.76282300 -1.06112600
C 0.10731300 -2.52974800 -2.34270500
C 1.22909000 -3.21224200 -2.82597800
H 2.73332700 -4.70886000 -2.39780300
H 1.78604500 -5.23409400 -0.15324400
H -0.16768200 -4.01242600 0.69076600
H -0.33696600 -1.76506500 -2.98593500
H 1.62821700 -2.97762400 -3.81364500

C	1.41677500	-1.06765600	2.35343800	H	-1.05457400	4.76614100	1.69040400
H	0.94091600	-0.07928000	2.28903300	H	-1.43873300	4.67372000	-0.02623300
H	0.77562100	-1.78242800	1.81107600	H	-1.98781000	3.39460700	1.06611300
H	1.42163500	-1.36740300	3.41189100	C	0.51406300	2.74979800	2.03768300
C	3.38417000	-2.46889500	1.99679600	H	-0.25823600	2.05656700	2.41232800
H	4.46744500	-2.55120300	1.86598100	H	1.47690500	2.21711300	2.03178300
H	3.16409900	-2.80715200	3.02011100	H	0.59488600	3.57315100	2.76214700
H	2.91120200	-3.18566000	1.30683200	C	-3.71156300	-0.22884600	-2.03147200
C	4.90802100	-1.54928900	-0.61351000	H	-2.99116000	0.56580800	-2.28022300
H	5.73179900	-1.27487100	-1.28902600	H	-3.22276300	-1.19996300	-2.21307300
H	5.36347900	-2.01576500	0.26487000	H	-4.54998900	-0.14287400	-2.73821200
H	4.30802000	-2.32018100	-1.12412000	C	-4.88664700	1.27770000	-0.49768700
C	3.76669100	0.34222800	-1.64612800	H	-4.13461400	2.08132800	-0.47265600
H	3.18864500	-0.32822200	-2.30461600	H	-5.52770300	1.44869800	-1.37540600
H	3.20047100	1.27789600	-1.52988400	H	-5.52440100	1.39754300	0.38462900
H	4.70546800	0.58303200	-2.16568700	C	-3.82808000	0.82869400	2.47203700
C	-1.43385100	3.09467000	-2.12448700	H	-4.81960200	1.17823300	2.16886400
H	-1.57903500	3.01264600	-3.21184700	H	-3.86114000	0.67469400	3.56106500
H	-2.27475700	2.57000100	-1.64527200	H	-3.11713400	1.64817800	2.27716800
H	-1.53127800	4.15632000	-1.87623900	C	-2.10630500	-0.90385100	2.48322800
C	0.05462100	1.19322800	-2.53276100	H	-1.71611200	-1.85064300	2.07692700
H	-0.72633400	0.46471000	-2.25414800	H	-1.30732300	-0.14757700	2.39516200
H	-0.04796200	1.39377000	-3.60945800	H	-2.29456600	-1.04984700	3.55704800
H	1.02827700	0.70872900	-2.37322200	Li	-1.50370600	0.95519400	0.13165500
C	-1.14871900	4.07365000	0.84091900				

3-e)

Cartesian Coordinates

C	-3.17506900	-1.35670300	1.63641800	C	-5.14896300	0.20596300	0.12965900
C	-4.11491600	-0.67164700	-0.59524300	C	-5.49314600	-0.30907000	1.51756500

C	-4.22104800	-0.47177400	2.33380000
H	-4.72967800	1.22485400	0.22661500
H	-6.05594000	0.29633900	-0.49081500
H	-6.18228100	0.38518100	2.02071000
H	-6.03092100	-1.26852600	1.44837200
H	-3.77760600	0.52679600	2.50054100
H	-4.44634200	-0.88522500	3.33080600
N	-2.91958000	-0.87948500	0.25499400
Cu	-1.49507500	-1.88905900	-0.57666900
C	-0.19496600	2.62185200	-1.69428900
C	-0.56629800	3.18395300	0.73676200
C	-1.79192000	4.02033200	0.32857400
C	-1.68046100	4.59715800	-1.07199100
C	-1.42157900	3.47441900	-2.06334800
H	-2.68563500	3.36892000	0.36715200
H	-1.95624800	4.81801700	1.07147800
H	-2.60402300	5.13237700	-1.33711900
H	-0.87553500	5.34830000	-1.11520300
H	-2.31185800	2.82332100	-2.09781400
H	-1.29110900	3.87434600	-3.08239400
N	-0.27424900	2.14810300	-0.28649500
C	2.96678900	-0.44999600	1.91677500
C	4.01672300	0.34492000	-0.23989100
C	5.18722600	-0.62406400	0.00450500
C	5.43458400	-0.90355700	1.47670600
C	4.15206700	-1.40997700	2.11364500
H	4.95857500	-1.58157000	-0.49984700
H	6.09461800	-0.22582200	-0.47852200
H	6.23836800	-1.64520800	1.59366400
H	5.78726000	0.00567000	1.98958900
H	3.89240300	-2.38322800	1.65675500
H	4.29404500	-1.59843500	3.19036700
N	2.79780700	-0.10145000	0.48330800

Cu	1.25749200	1.03951700	0.15120100
Li	1.91016800	-1.53576900	-0.49887700
C	2.63126700	-3.82043200	-2.01324800
C	2.03808900	-4.20198500	-0.80837400
C	0.79139800	-3.67960700	-0.44648000
C	0.08091100	-2.75544700	-1.24843200
C	0.71055700	-2.41603600	-2.46760100
C	1.95207500	-2.93406600	-2.85097800
H	3.60912800	-4.20897500	-2.29565600
H	2.55290700	-4.89800400	-0.14469700
H	0.36441200	-3.99494600	0.51025300
H	0.22398500	-1.70438700	-3.13997900
H	2.40109000	-2.62968800	-3.79747800
C	3.71581600	0.30890200	-1.73965400
H	3.40355400	-0.69507700	-2.07382800
H	2.92674100	1.02240800	-2.01709300
H	4.61243700	0.56678600	-2.32172500
C	4.46942400	1.78155600	0.07984300
H	4.92367800	1.88057800	1.07195500
H	5.21854600	2.12258500	-0.65121200
H	3.61574900	2.47406100	0.03760500
C	3.12322100	0.75499000	2.86145300
H	3.05707400	0.43170000	3.91176000
H	4.07831100	1.27817800	2.74576700
H	2.32234700	1.48801700	2.68418600
C	1.70458900	-1.18255700	2.36564500
H	0.82076300	-0.53235900	2.28985500
H	1.51354200	-2.08541100	1.76083800
H	1.78822200	-1.51166400	3.41177200
C	0.61235900	4.11569500	1.07083700
H	0.89160400	4.77499200	0.24270800
H	0.36681200	4.75905100	1.92983500
H	1.50258100	3.52534400	1.33609600

C	-0.92692500	2.46731800	2.03757200	H	-2.02453600	-1.49670700	3.48060400
H	-0.10805500	1.81432300	2.37954300	C	-3.59813500	-2.83545100	1.74869400
H	-1.13564300	3.18812700	2.84096900	H	-3.54583900	-3.16771700	2.79716000
H	-1.83866900	1.85491700	1.93020100	H	-4.61917000	-3.02976300	1.40418800
C	1.07223600	3.42623500	-2.05246300	H	-2.92130700	-3.47231000	1.15817000
H	1.19571500	3.47460100	-3.14541700	C	-4.78933900	-1.96100400	-1.10216500
H	1.04795200	4.46075900	-1.69211800	H	-5.32648300	-2.51057500	-0.32231200
H	1.97150300	2.95450700	-1.63284700	H	-5.52207200	-1.72628500	-1.88971200
C	-0.18977200	1.38872900	-2.59981700	H	-4.03701300	-2.63994600	-1.53083100
H	0.72516700	0.79168100	-2.46175400	C	-3.67088200	0.08307700	-1.84544200
H	-1.04836300	0.73015400	-2.40213300	H	-3.20688500	1.04927400	-1.58897400
H	-0.23901300	1.68207700	-3.65891500	H	-2.95065700	-0.50659300	-2.43563700
C	-1.86948600	-1.24564100	2.42087000	H	-4.52796300	0.30936200	-2.49597500
H	-1.10697800	-1.93483200	2.02417500	Li	-1.58027500	0.63950400	0.03421900
H	-1.45944800	-0.22550800	2.38673800				

3-f)

Cartesian Coordinates

C	-3.24932900	-1.10352700	1.69485400	Cu	-1.59426500	-1.90182700	-0.47220800
C	-4.11979300	-0.52174600	-0.59146200	C	-0.05330700	2.53843900	-1.78310900
C	-5.07818900	0.49678000	0.04843400	C	-0.33864700	3.19669500	0.62428800
C	-5.46379100	0.13292200	1.47335700	C	-1.55574700	4.05027000	0.22179100
C	-4.21224000	-0.07575700	2.31158600	C	-1.48885900	4.56337000	-1.20573300
H	-4.57681300	1.48258400	0.05969600	C	-1.27438400	3.39793300	-2.15743100
H	-5.97543400	0.60773100	-0.58284700	H	-2.46397000	3.42659300	0.32761900
H	-6.08759400	0.92572800	1.91193400	H	-1.66901200	4.88488100	0.93303000
H	-6.08597700	-0.77665800	1.48098300	H	-2.41610300	5.09688700	-1.46143500
H	-3.68136100	0.88971700	2.40224300	H	-0.67995100	5.30434500	-1.30794600
H	-4.47632900	-0.38583000	3.33626600	H	-2.17729400	2.76393400	-2.14683700
N	-2.94794900	-0.75228200	0.28572700	H	-1.16009200	3.75594100	-3.19412000

N	-0.11769800	2.10695000	-0.36059600	H	4.82550200	-1.75188400	2.19022700
C	4.04487500	0.01563900	-0.27056700	C	5.11444600	-1.09192400	-0.37630500
C	2.93566000	-0.61157700	1.89204600	H	5.85610400	-0.82020600	-1.14187600
C	3.54758600	0.62594800	2.56706800	H	5.67164100	-1.26788700	0.54827100
C	4.83965100	1.08271600	1.89935900	H	4.66183300	-2.04882300	-0.68025900
C	4.65423200	1.25853500	0.39642400	C	3.68892300	0.35357100	-1.71734100
H	2.80831200	1.44539100	2.51652900	H	3.30016800	-0.53077500	-2.25255100
H	3.72057800	0.42348800	3.63773100	H	2.92912700	1.14254100	-1.77692000
H	5.17984900	2.02741600	2.34830500	H	4.57491500	0.70211500	-2.26718500
H	5.64419800	0.35564500	2.09765600	C	0.88034200	4.10344800	0.87065600
H	3.97780500	2.11298500	0.21396000	H	1.14803500	4.71964900	0.00657400
H	5.61657100	1.50961100	-0.08122500	H	0.68885600	4.78781500	1.71149900
N	2.79701700	-0.39803300	0.42663300	H	1.75975100	3.49286500	1.12635500
Cu	1.34125200	0.88782800	0.07162700	C	-0.67551700	2.56858000	1.97494400
Li	1.86671800	-1.79805900	-0.51029300	H	0.15214500	1.95260800	2.35671300
C	2.42870200	-4.03950400	-1.90496700	H	-0.88154800	3.34587800	2.72466500
C	1.83571100	-4.38128400	-0.68781900	H	-1.58212700	1.94328100	1.92346400
C	0.61366500	-3.80704700	-0.31792300	C	1.21418900	3.32702100	-2.18710700
C	-0.07528500	-2.87425700	-1.12882100	H	1.39852300	3.22600900	-3.26760900
C	0.55082100	-2.57883600	-2.36225000	H	1.13600000	4.40155500	-1.98354100
C	1.77201500	-3.14144100	-2.74959100	H	2.10249700	2.96181500	-1.65647600
H	3.38988200	-4.46531700	-2.19058400	C	-0.08341900	1.27844000	-2.65104600
H	2.33497100	-5.08270300	-0.01811000	H	0.83188900	0.67947700	-2.52810600
H	0.19279600	-4.08451500	0.65273400	H	-0.93825300	0.63093700	-2.40463000
H	0.08161500	-1.86170400	-3.04117500	H	-0.16860500	1.54127300	-3.71593600
H	2.22187200	-2.86610500	-3.70448200	C	-1.94119300	-1.06033100	2.48149100
C	1.54018700	-0.84822100	2.46234600	H	-1.25158200	-1.85214700	2.14812400
H	0.86406900	-0.01061200	2.24111500	H	-1.42527400	-0.09558700	2.37236200
H	1.08828400	-1.76031400	2.03733200	H	-2.12401000	-1.20914400	3.55597400
H	1.57184800	-0.97322100	3.55464400	C	-3.80832000	-2.52465500	1.91132000
C	3.74179800	-1.86753600	2.28375400	H	-3.77287200	-2.78755700	2.97990900
H	3.54399000	-2.12308100	3.33515700	H	-4.84782800	-2.64542900	1.58960900
H	3.44245600	-2.73249400	1.67175700	H	-3.20173200	-3.26045300	1.36154100

C	-4.89890600	-1.78916900	-0.99364700	H	-3.06661900	1.02229400	-1.72190300
H	-5.49475800	-2.21526900	-0.18017500	H	-2.94458100	-0.61367100	-2.43187700
H	-5.59640600	-1.56402200	-1.81514400	H	-4.44733400	0.32530100	-2.57124200
H	-4.20443200	-2.56788900	-1.34254700	Li	-1.51363400	0.67803200	0.00522200
C	-3.61248500	0.08227900	-1.89818600				

3-g)

Cartesian Coordinates

C	-3.31550800	-0.98986500	1.66704700	H	1.68765700	3.74137200	0.72753300
C	-4.14497100	-0.66249000	-0.68693400	H	0.64357900	5.12098200	1.09913100
C	-5.09030900	0.44360900	-0.18815600	N	-0.35138400	2.13750400	-0.30469000
C	-5.49652800	0.26205800	1.26682800	C	2.91169600	-0.48040700	1.89665500
C	-4.26228300	0.12318300	2.14581200	C	3.95223800	0.16882300	-0.30542700
H	-4.57150600	1.41558800	-0.29230800	C	5.02591100	-0.91432300	-0.09179800
H	-5.98036400	0.49376500	-0.83712600	C	5.29417800	-1.21632600	1.37263600
H	-6.10518200	1.11570300	1.59962700	C	3.99043800	-1.56365900	2.07189700
H	-6.14150600	-0.62501900	1.37431900	H	4.68450400	-1.84371100	-0.58650200
H	-3.70708500	1.08076500	2.13374000	H	5.95419100	-0.61367500	-0.60489700
H	-4.55002900	-0.05754300	3.19485400	H	6.00925900	-2.04705600	1.46452300
N	-2.99544800	-0.80467400	0.23403500	H	5.77467100	-0.35298900	1.86022900
Cu	-1.58396000	-1.94507000	-0.41406400	H	3.60483600	-2.51300600	1.65415500
C	-0.41177900	3.26906600	0.66057400	H	4.15802900	-1.74242000	3.14686200
C	-0.27987000	2.54593700	-1.73632500	N	2.72167100	-0.15957100	0.45860900
C	0.88739600	3.51954700	-1.97294600	Cu	1.20640000	1.00965000	0.10824300
C	0.86568000	4.70607900	-1.01673400	Li	1.78545300	-1.62970200	-0.42014800
C	0.75129000	4.24893400	0.43204900	C	2.47694700	-4.04468500	-1.80686900
H	1.83490900	2.96860200	-1.83760800	C	1.91499700	-4.34474700	-0.56474900
H	0.87480000	3.87101800	-3.01895300	C	0.68845700	-3.78117300	-0.19639500
H	1.77517200	5.31049000	-1.14936300	C	-0.03414000	-2.89623300	-1.03079200
H	0.02765400	5.37761600	-1.26504800	C	0.56344400	-2.63982800	-2.28667700

C	1.78663900	-3.19715000	-2.67475600	H	0.08062200	1.54827100	-3.63804600
H	3.44007500	-4.46513100	-2.09416000	H	0.84668900	0.73900100	-2.25545600
H	2.43972500	-5.00878900	0.12351100	C	-1.74924600	4.03610500	0.65370000
H	0.28812000	-4.03044300	0.79048300	H	-1.82011000	4.66898000	1.55080000
H	0.06711500	-1.96146200	-2.98640500	H	-1.88495700	4.69485500	-0.20875900
H	2.21123300	-2.95575000	-3.65024400	H	-2.59929100	3.33604600	0.67643000
C	3.61227100	0.16905800	-1.79691900	C	-0.29386100	2.70638400	2.07579100
H	3.12930200	-0.76931800	-2.11948300	H	-1.17547900	2.10037300	2.33952300
H	2.94832900	1.00336500	-2.06276900	H	0.60036800	2.07760100	2.19531600
H	4.52712200	0.27372500	-2.39821600	H	-0.22966400	3.52033800	2.81239100
C	4.54754500	1.55652600	-0.00931000	C	-2.01069700	-0.87449000	2.45350800
H	5.32020200	1.80975200	-0.75157000	H	-1.33148800	-1.71198700	2.22721200
H	3.76257700	2.32549100	-0.06261400	H	-1.47400400	0.06129200	2.23038700
H	5.01482100	1.62882400	0.97821200	H	-2.20126600	-0.88028400	3.53686800
C	3.25694100	0.72018000	2.79925500	C	-3.89872000	-2.36641900	2.04056500
H	3.07806700	0.46859000	3.85574300	H	-3.30544800	-3.16802000	1.57609500
H	4.30374000	1.03425900	2.72214800	H	-3.86800300	-2.50911800	3.13186700
H	2.63459500	1.59050200	2.54840000	H	-4.94050300	-2.50181000	1.73241200
C	1.59632700	-1.05322200	2.42318400	C	-4.94150300	-1.95594800	-0.94331700
H	0.79334400	-0.30197400	2.40223100	H	-5.56116000	-2.26504000	-0.09521000
H	1.25633700	-1.92311400	1.83597700	H	-5.61815200	-1.82397500	-1.80157600
H	1.70652200	-1.39476900	3.46281100	H	-4.25539000	-2.78371000	-1.17566600
C	-1.57444400	3.18227700	-2.29175300	C	-3.60044100	-0.23376300	-2.04843200
H	-1.65658400	4.25590700	-2.09241500	H	-3.02428300	0.70158900	-1.97946400
H	-1.61182600	3.06513800	-3.38476600	H	-2.94575700	-1.00806800	-2.48144100
H	-2.47234100	2.70331100	-1.87662600	H	-4.41874300	-0.05040300	-2.75983200
C	-0.04941500	1.28804900	-2.57733000	Li	-1.65600900	0.67598000	0.00161800
H	-0.90310200	0.59447800	-2.51182900				

3-h)

Cartesian Coordinates

C	-3.37596800	-0.49732000	1.76266100	H	5.71732700	-0.32659700	1.99067600
C	-4.20201800	-0.60329700	-0.61656500	H	4.24300300	1.87328200	0.44124100
C	-5.24479600	0.47587900	-0.28552000	H	5.78607300	1.13415500	-0.02076700
C	-5.67313300	0.44702300	1.17274900	N	2.77188700	-0.49292300	0.35550800
C	-4.44854300	0.56348800	2.06483200	Cu	1.36112600	0.83096300	0.01875300
H	-4.80326000	1.46519300	-0.50629200	Li	1.78207000	-1.88223600	-0.54652800
H	-6.11595400	0.36287000	-0.95170200	C	2.07604100	-4.22945900	-1.88436600
H	-6.37315900	1.26935900	1.38176000	C	1.57751400	-4.50738300	-0.61041000
H	-6.22482200	-0.48092400	1.39415300	C	0.43884500	-3.84278500	-0.14093300
H	-4.00037600	1.56243900	1.90982200	C	-0.25947000	-2.87968900	-0.90464200
H	-4.73006500	0.50866700	3.12945200	C	0.26214600	-2.65687000	-2.20164700
N	-3.05078100	-0.52334100	0.31676100	C	1.40315100	-3.30522800	-2.68712100
Cu	-1.68483300	-1.78864500	-0.21582100	H	2.97573800	-4.72550400	-2.24658400
C	0.07118600	3.31284100	0.54512800	H	2.08944800	-5.22941200	0.02715200
C	-0.29581400	2.39538400	-1.76200900	H	0.09846900	-4.06959200	0.87288500
C	0.74198200	3.38152900	-2.32277200	H	-0.22230600	-1.92653200	-2.85572500
C	0.85249200	4.64960700	-1.48983200	H	1.77566300	-3.08070800	-3.68741600
C	1.10563400	4.29443200	-0.03356200	C	1.48934500	-0.92136500	2.39163500
H	1.72574400	2.88235400	-2.34182400	H	0.96377100	0.03967600	2.29962100
H	0.49154500	3.62290900	-3.36989700	H	0.87546400	-1.68902700	1.88896600
H	1.66698700	5.28231000	-1.87220900	H	1.52866600	-1.18024600	3.46002900
H	-0.06267600	5.25683200	-1.58293100	C	3.51654100	-2.24163100	2.04750700
H	2.10076800	3.82007400	0.04439800	H	3.33702200	-2.55178900	3.08753700
H	1.14015100	5.20488400	0.58796400	H	3.06235200	-3.00628900	1.39707800
N	-0.08141000	2.10849000	-0.31532500	H	4.59903400	-2.27794400	1.89144100
C	4.04156200	-0.12619800	-0.32623000	C	4.95830400	-1.33043200	-0.62572200
C	2.89552800	-0.85059400	1.79677200	H	5.75869300	-1.03440100	-1.32003000
C	3.69755000	0.20220900	2.57818400	H	5.44758600	-1.75033400	0.25815400
C	5.03139600	0.53387800	1.92485200	H	4.39195500	-2.14417200	-1.10813600
C	4.82005200	0.93138800	0.47151500	C	3.70143200	0.46863600	-1.69172100
H	3.09455800	1.12403700	2.63945600	H	3.14494300	-0.25003100	-2.31707600
H	3.84791300	-0.14288000	3.61496900	H	3.09015000	1.37794100	-1.59210200
H	5.52605000	1.34985000	2.47184100	H	4.61667800	0.73955200	-2.23794200

C	-1.70581900	2.94680800	-2.08802100	H	-1.29118500	-0.80387800	2.34188400
H	-1.78461900	4.03223600	-1.96253400	H	-1.76454800	0.91899000	2.22267100
H	-1.97030500	2.73312900	-3.13414100	H	-2.28945600	-0.04149100	3.59848200
H	-2.48587700	2.49799600	-1.45401800	C	-3.79769200	-1.85319300	2.35844500
C	-0.15747300	1.07848000	-2.52956000	H	-3.07232200	-2.63216800	2.07784400
H	-0.87469800	0.31613100	-2.18016300	H	-3.83011000	-1.79899400	3.45769900
H	-0.34264700	1.22979500	-3.60333900	H	-4.78589000	-2.18630500	2.02531300
H	0.85119900	0.65553800	-2.41724500	C	-4.89387200	-1.98034700	-0.67707000
C	-1.25824000	4.04543500	0.81118600	H	-5.48135300	-2.21746300	0.21595100
H	-1.12037700	4.82089400	1.57937400	H	-5.58438800	-2.02236900	-1.53352400
H	-1.67720800	4.54023100	-0.06989400	H	-4.14766600	-2.77885500	-0.80601000
H	-2.01842500	3.34244800	1.18931700	C	-3.68783700	-0.33723100	-2.03131700
C	0.58254900	2.88461200	1.91950300	H	-3.17917100	0.63384400	-2.10084100
H	-0.09685600	2.16583100	2.40127600	H	-2.98237700	-1.11940500	-2.35752200
H	1.57759000	2.41977200	1.85050100	H	-4.52001300	-0.32357500	-2.75031200
H	0.67103300	3.75522500	2.58583500	Li	-1.57204500	0.82104700	0.06533400
C	-2.10988800	-0.08807000	2.51494800				

Structure optimization for 4

4-a)

Cartesian Coordinates

Cu -0.74109500 1.89403000 0.00005900	H -1.37103600 1.17661700 2.48194600
Li -1.65665800 -0.73887500 -0.00015000	H -2.07908600 -0.44320500 2.22934800
N -2.45387800 1.01366100 -0.00048600	C 0.97472600 2.77928200 0.00081000
C -3.19354300 1.19226800 -1.27051400	C 1.63256100 3.15039600 -1.19264600
C -3.47997300 2.65677100 -1.64460900	H 1.17779500 2.89892200 -2.15594700
H -3.86341200 2.72614900 -2.67430000	C 2.84681000 3.84039000 -1.20082500
H -2.55719200 3.25384400 -1.58503400	H 3.31587800 4.10835500 -2.14819300
H -4.22193900 3.13020800 -0.99207800	C 3.46111100 4.18267800 0.00215800
C -2.31870200 0.62269300 -2.39140400	H 4.41237300 4.71395300 0.00267000
H -2.83441700 0.68226300 -3.36075900	C 2.84589700 3.83969500 1.20447600
H -2.07784000 -0.44301500 -2.23017200	H 3.31425600 4.10710300 2.15235400
H -1.36971700 1.17685600 -2.48236800	C 1.63165300 3.14972300 1.19497900
C -4.50743600 0.39372200 -1.24552300	H 1.17615500 2.89769500 2.15780800
H -5.08626300 0.60717000 -2.15905900	Cu 0.74106600 -1.89393100 -0.00012300
H -4.26417900 -0.68552800 -1.27436700	Li 1.65672200 0.73896500 0.00007200
C -5.33782400 0.66818700 -0.00129100	N 2.45388500 -1.01360000 -0.00051100
H -6.23953100 0.03862500 -0.00157900	C 3.19418200 -1.19230400 1.26913900
H -5.69743100 1.70994600 -0.00131200	C 3.48069200 -2.65683600 1.64304600
C -4.50810500 0.39354800 1.24334600	H 3.86482200 -2.72625600 2.67247700
H -4.26481700 -0.68571800 1.27213200	H 2.55779600 -3.25380100 1.58410900
H -5.08742600 0.60680500 2.15661100	H 4.22215000 -3.13036800 0.99001300
C -3.19426000 1.19213300 1.26915000	C 2.31993500 -0.62270900 2.39050100
C -3.48094700 2.65659100 1.64321600	H 2.83607500 -0.68249000 3.35961600
H -3.86497900 2.72586100 2.67269300	H 2.07919100 0.44306900 2.22954700
H -4.22255300 3.13006400 0.99030700	H 1.37088700 -1.17670700 2.48182400
H -2.55815100 3.25369800 1.58423000	C 4.50809900 -0.39383000 1.24349500
C -2.31999700 0.62249000 2.39047500	H 5.08735200 -0.60726000 2.15676500
H -2.83621300 0.68203300 3.35956800	H 4.26490600 0.68543500 1.27240000

C	5.33786800	-0.66838800	-0.00113000	H	1.36982100	-1.17639900	-2.48244000
H	6.23961900	-0.03888800	-0.00129200	H	2.07806900	0.44337200	-2.22998200
H	5.69740600	-1.71017100	-0.00126000	C	-0.97473800	-2.77922100	0.00065200
C	4.50757100	-0.39370200	-1.24537600	C	-1.63157400	-3.14966400	1.19487200
H	4.26442800	0.68558900	-1.27410300	H	-1.17604600	-2.89757900	2.15765200
H	5.08642100	-0.60709600	-2.15890700	C	-2.84576300	-3.83972900	1.20445900
C	3.19359900	-1.19210900	-1.27052600	H	-3.31404100	-4.10716000	2.15236900
C	3.47992700	-2.65658700	-1.64479700	C	-3.46103800	-4.18276200	0.00218800
H	3.86339000	-2.72586300	-2.67448600	H	-4.41227000	-4.71409100	0.00277000
H	4.22184300	-3.13015500	-0.99231000	C	-2.84684200	-3.84044800	-1.20084200
H	2.55710300	-3.25360500	-1.58532400	H	-3.31596700	-4.10844000	-2.14817700
C	2.31884600	-0.62231400	-2.39137100	C	-1.63261900	-3.15040700	-1.19275300
H	2.83458900	-0.68179300	-3.36072000	H	-1.17791600	-2.89893300	-2.15610500

4-b)

Cartesian Coordinates

Cu	-0.91773500	-1.75379900	0.02098700	H	-3.37650900	-3.06397800	-1.30447100
Li	-1.62515800	0.96969900	-0.01628900	C	-4.97876000	-2.32729600	-0.07712700
N	-2.55155500	-0.71021000	-0.04837000	H	-5.48663300	-3.30267300	-0.06758400
C	-3.27211700	-0.91447300	-1.32937200	H	-5.78230000	-1.57360600	-0.11854700
C	-4.18574700	0.26377200	-1.72052600	C	-4.15711700	-2.15633700	1.19340200
H	-4.51265500	0.16221800	-2.76607700	H	-3.45113900	-3.00176600	1.27438400
H	-3.65232000	1.22552300	-1.63630800	H	-4.80594200	-2.19591400	2.08443100
H	-5.09197000	0.33864100	-1.11121900	C	-3.34221300	-0.85408300	1.19962600
C	-2.22704500	-1.01540100	-2.44315700	C	-4.27205900	0.34290500	1.48240800
H	-2.70972800	-1.14259300	-3.42308300	H	-4.65821800	0.29168200	2.51128000
H	-1.55082600	-1.87190300	-2.29071900	H	-5.14150300	0.38971200	0.81920000
H	-1.60773000	-0.10316700	-2.49621400	H	-3.73293000	1.30091500	1.38508700
C	-4.08574300	-2.21735600	-1.30561600	C	-2.36039900	-0.90412300	2.37345500
H	-4.68280300	-2.30256800	-2.22902900	H	-2.89746400	-0.98309700	3.32988000

H	-1.73894700	0.00760400	2.42098600	H	4.17380100	-1.00754300	-1.33970100
H	-1.68209900	-1.76902300	2.29905900	C	5.38222100	0.28492900	-0.12657000
C	0.71402600	-2.78828900	0.09550600	H	6.23514400	-0.40916600	-0.14130500
C	1.30283800	-3.17501600	1.31975000	H	5.81650900	1.29737200	-0.15677900
H	0.85457800	-2.83955400	2.26014000	C	4.57256100	0.09245900	1.14613200
C	2.43940000	-3.98343600	1.38885300	H	4.24981100	-0.96464200	1.20040100
H	2.85486700	-4.25908600	2.35878900	H	5.19333600	0.27548900	2.03850400
C	3.04468400	-4.43507700	0.21780700	C	3.32344100	0.98780600	1.19616800
H	3.93551500	-5.06074400	0.26440900	C	3.72874600	2.43295300	1.53424100
C	2.49859500	-4.07821800	-1.01336300	H	4.15423000	2.48946600	2.54808900
H	2.96050300	-4.42870000	-1.93703400	H	4.47745800	2.84231100	0.84729000
C	1.36103400	-3.26942000	-1.06417700	H	2.84953900	3.09437600	1.49797000
H	0.95895000	-3.01203600	-2.04905200	C	2.44514700	0.50463200	2.35442700
Cu	0.89768900	1.86235700	-0.00803500	H	2.99436300	0.54396900	3.30624700
Li	1.57367800	-0.82328800	0.02007700	H	1.54322300	1.12959600	2.46291100
N	2.53225000	0.84481600	-0.04746300	H	2.12174600	-0.54310100	2.22350900
C	3.24371000	0.94345100	-1.34198800	C	-0.72358200	2.90735100	0.05569500
C	3.62552800	2.37556100	-1.75514400	C	-1.38635500	3.36201400	-1.10577500
H	3.97947800	2.39715900	-2.79744200	H	-1.00136500	3.07649100	-2.09005500
H	2.75177000	3.04072200	-1.67936800	C	-2.51864900	4.17866500	-1.05526100
H	4.42106000	2.80450600	-1.13584500	H	-2.99577500	4.50780800	-1.97905000
C	2.29470000	0.42070700	-2.42443200	C	-3.04087500	4.56954600	0.17588000
H	2.78581300	0.41557800	-3.40829600	H	-3.92725000	5.20142600	0.22186100
H	1.97186000	-0.61747300	-2.22960000	C	-2.41946500	4.14243200	1.34787200
H	1.39228700	1.04908200	-2.50431800	H	-2.81894300	4.44300200	2.31705500
C	4.49588100	0.05082500	-1.33989400	C	-1.29064400	3.32331600	1.28068700
H	5.05989800	0.20540500	-2.27433200	H	-0.83025700	3.00382300	2.22076200

4-c)

Cartesian Coordinates

Cu -1.09032300 1.69440800 -0.02934000
Li -1.52351100 -1.06675100 -0.03203900
N -2.61315700 0.50283300 0.13171900
C -3.25416200 0.59888800 1.46620300
C -4.02471200 -0.67147200 1.87745300
H -4.28233800 -0.63167600 2.94629900
H -3.41208000 -1.57495500 1.72120300
H -4.96226000 -0.81409700 1.33091700
C -2.14496400 0.76314500 2.50740400
H -2.56524700 0.82154300 3.52198400
H -1.55856100 1.68015200 2.33552300
H -1.44773100 -0.09263400 2.48811000
C -4.18437900 1.81847800 1.54722300
H -4.71505500 1.82092900 2.51406000
H -3.55898600 2.72854100 1.52341800
C -5.17421100 1.87508700 0.39151500
H -5.77187800 2.79622800 0.45254100
H -5.89691700 1.04578600 0.46482800
C -4.43807700 1.82055500 -0.94016500
H -3.82550900 2.73375300 -1.04233800
H -5.15290600 1.82064900 -1.78009500
C -3.50351100 0.60616700 -1.05202600
C -4.32931900 -0.66887300 -1.31423500
H -4.79855600 -0.62234000 -2.30820700
H -5.13464900 -0.82672000 -0.58996200
H -3.69130500 -1.56927400 -1.29817400
C -2.62035500 0.79217700 -2.28913100
H -3.23129000 0.83796500 -3.20243900
H -1.91071600 -0.04537100 -2.41177500
H -2.03458600 1.72338800 -2.23318400
C 0.41927800 2.88230000 -0.24024200
C 0.90915500 3.23460200 -1.51778000
H 0.45850800 2.78465400 -2.40785900

C 1.94878800 4.14858900 -1.70134800
H 2.28874400 4.39354100 -2.70818700
C 2.55717000 4.74243300 -0.59714400
H 3.37431300 5.45014200 -0.73307400
C 2.11245900 4.41817000 0.68271400
H 2.58111800 4.87545200 1.55490900
C 1.06854500 3.50457800 0.84892000
H 0.74554700 3.27550800 1.86951100
Cu 1.09033700 -1.69444800 -0.02933800
Li 1.52350300 1.06667800 -0.03254500
N 2.61316000 -0.50285800 0.13167500
C 3.50356900 -0.60627600 -1.05202200
C 4.32934300 0.66876800 -1.31431900
H 4.79862200 0.62216100 -2.30826800
H 3.69130400 1.56915600 -1.29836700
H 5.13463600 0.82671200 -0.59002600
C 2.62047100 -0.79244000 -2.28914600
H 3.23144600 -0.83829800 -3.20242500
H 2.03472700 -1.72366200 -2.23313100
H 1.91080600 0.04507000 -2.41191700
C 4.43817700 -1.82061700 -0.94001000
H 5.15303900 -1.82076400 -1.77991100
H 3.82564700 -2.73384800 -1.04211800
C 5.17425700 -1.87498900 0.39170600
H 5.77196200 -2.79609800 0.45284600
H 5.89692300 -1.04564900 0.46497200
C 4.18437100 -1.81831300 1.54736400
H 3.55901700 -2.72840400 1.52361400
H 4.71500400 -1.82065300 2.51422500
C 3.25410600 -0.59876700 1.46619500
C 4.02458200 0.67166300 1.87736500
H 4.28217600 0.63196800 2.94622200
H 4.96214300 0.81428400 1.33084700

H	3.41190800	1.57509700	1.72101400	C	-2.11242200	-4.41823100	0.68275000
C	2.14487300	-0.76298400	2.50736500	H	-2.58103200	-4.87556200	1.55494500
H	2.56512100	-0.82128000	3.52196500	C	-2.55720900	-4.74241400	-0.59710100
H	1.44760700	0.09276100	2.48796400	H	-3.37436700	-5.45010700	-0.73302700
H	1.55852300	-1.68003600	2.33553900	C	-1.94888500	-4.14851000	-1.70130600
C	-0.41927700	-2.88232300	-0.24021700	H	-2.28890500	-4.39339600	-2.70813800
C	-1.06848400	-3.50466200	0.84894800	C	-0.90923500	-3.23454100	-1.51774600
H	-0.74541500	-3.27566400	1.86953300	H	-0.45864700	-2.78453200	-2.40782300

Structure optimization for 5

5-a)

Cartesian Coordinates

C	3.92505600	-0.78826000	0.63215600	C	-5.23752100	-0.68214600	0.17754400
C	3.06234300	-1.10258500	-1.72692000	C	-5.56185400	-0.94030300	-1.28404300
C	3.86449600	-2.40961700	-1.82770000	C	-4.30512900	-1.38833300	-2.01088400
C	5.10218000	-2.41704900	-0.94618900	H	-4.94799700	-1.64021100	0.64894300
C	4.71938400	-2.09714400	0.48895700	H	-6.12804400	-0.32389300	0.71973800
H	3.20505700	-3.24184400	-1.52384100	H	-6.34612800	-1.70664700	-1.37047300
H	4.13611700	-2.58648400	-2.88166600	H	-5.97546800	-0.03288900	-1.75276700
H	5.59588300	-3.39858700	-0.99564100	H	-3.98953600	-2.36519500	-1.59900200
H	5.84396400	-1.69099700	-1.31674100	H	-4.50715700	-1.55187000	-3.08217400
H	4.09558500	-2.91865600	0.88357400	N	-2.90114900	-0.08178400	-0.42645200
H	5.61711000	-2.04533600	1.12682700	Cu	-1.34807600	1.04016800	-0.12856700
N	2.75756400	-0.78434400	-0.29979900	Li	-1.94349900	-1.54080400	0.43471500
Cu	1.28636300	-1.88874900	0.38522900	C	-2.70382100	-4.01438500	1.92911500
Cu	1.46920600	0.66639000	-0.03531000	C	-2.17863500	-4.33181200	0.67564200
C	0.24600900	2.56894000	1.70657500	C	-0.96654000	-3.76988800	0.26152300
C	0.43720600	3.22742400	-0.73256700	C	-0.22549600	-2.86540200	1.05728000
C	1.75251600	3.95684400	-0.41596400	C	-0.78472600	-2.59314000	2.32744100
C	1.83890400	4.43857800	1.02492800	C	-1.99144300	-3.15117200	2.76228400
C	1.56883600	3.29642200	1.99445900	H	-3.65550100	-4.43474800	2.25236900
H	2.58771600	3.26054000	-0.61142400	H	-2.71995200	-5.01041900	0.01498800
H	1.87841500	4.80180100	-1.11286900	H	-0.59390100	-4.03657500	-0.73154300
H	2.83289000	4.86781300	1.21818200	H	-0.27038500	-1.89977500	2.99958000
H	1.12339500	5.25941800	1.19428200	H	-2.38634100	-2.89746000	3.74711800
H	2.39329500	2.56493400	1.92678300	C	-3.69698200	0.27878100	1.85047300
H	1.56161000	3.66704900	3.03295200	H	-3.29734100	-0.70592700	2.14794800
N	0.19594400	2.14533500	0.27127900	H	-2.94343800	1.04238700	2.09260000
C	-3.13859700	-0.39763800	-1.85703900	H	-4.57342700	0.46772800	2.48737200
C	-4.08626800	0.32021400	0.37177100	C	-4.59657300	1.74744200	0.10255200

H	-5.31201100	2.05421800	0.88102400	H	-1.88188200	3.08474000	1.75929300
H	-3.75921100	2.46077900	0.11177600	C	0.17424500	1.31857800	2.58440500
H	-5.10811600	1.85162800	-0.86051800	H	-0.82059600	0.85102900	2.53714200
C	-3.38467100	0.82637100	-2.75756400	H	0.90824600	0.55946400	2.28150700
H	-3.33784400	0.53913900	-3.81922200	H	0.36970700	1.57973700	3.63494400
H	-4.36084100	1.29598500	-2.59540800	C	3.42073900	-0.72334200	2.07366700
H	-2.61674100	1.59410100	-2.58106900	H	2.97274300	0.25381900	2.30216800
C	-1.88164500	-1.08093200	-2.39279900	H	2.67239200	-1.50560800	2.28209700
H	-1.00993800	-0.41285300	-2.33338700	H	4.25846500	-0.86998900	2.77081300
H	-1.63940900	-2.00015200	-1.83264700	C	4.86293300	0.41931200	0.46426700
H	-2.00973200	-1.37504600	-3.44464100	H	4.28124200	1.35215400	0.42383900
C	-0.71193000	4.24210700	-0.86047400	H	5.54702000	0.48491300	1.32348100
H	-0.79488300	4.93027700	-0.01430900	H	5.48574200	0.37483300	-0.43476000
H	-0.56366800	4.85905000	-1.75894000	C	3.80689400	0.01586700	-2.47995800
H	-1.67558100	3.72212100	-0.96682600	H	4.87780400	0.05762800	-2.25613100
C	0.57320700	2.58522400	-2.11118800	H	3.71759500	-0.13832700	-3.56544000
H	-0.35776800	2.08002200	-2.41217400	H	3.38173500	1.00123400	-2.24310000
H	0.80041800	3.34832300	-2.86941700	C	1.74463400	-1.31419900	-2.46924100
H	1.38439800	1.84316000	-2.13329800	H	1.13511700	-2.10126300	-1.99666400
C	-0.92864400	3.45703100	2.15989200	H	1.14510300	-0.39261300	-2.49282200
H	-0.99781800	3.44359500	3.25774100	H	1.93544000	-1.61645200	-3.50923300
H	-0.83151200	4.50698900	1.86613400				

5-b)

Cartesian Coordinates

C	-3.92369522	-0.71945876	-0.66238945	H	-3.30719753	-3.32510369	1.33703814
C	-3.05799044	-1.21220073	1.66696386	H	-4.19379785	-2.70952959	2.74202181
C	-3.92300174	-2.48221937	1.69763909	H	-5.70665041	-3.33686611	0.82838778
C	-5.16630813	-2.37890025	0.83040423	H	-5.86937240	-1.64073954	1.24937252
C	-4.77664489	-1.99658235	-0.58743688	H	-4.19312455	-2.82235961	-1.03155652

H	-5.67375072	-1.86757692	-1.21516457	C	0.18972755	-2.85462179	-1.23360230
N	-2.75189933	-0.81990921	0.25901839	C	0.75797893	-2.47102727	-2.47150915
Cu	-1.32013782	-1.92228522	-0.50183873	C	1.98569016	-2.96042233	-2.93051156
Cu	-1.41535697	0.60133533	0.06372792	H	3.67333818	-4.24457431	-2.49954798
C	-0.19001829	2.56137781	-1.60058265	H	2.71833226	-5.02532966	-0.33388639
C	-0.33200149	3.10678498	0.86188053	H	0.56677706	-4.15260446	0.46411538
C	-1.66739593	3.82737301	0.61196549	H	0.23750929	-1.73643024	-3.09275196
C	-1.81195092	4.35954054	-0.80652038	H	2.39003880	-2.61557049	-3.88322402
C	-1.53486667	3.26906276	-1.83248011	C	1.76807830	-0.94122931	2.40053581
H	-2.48489191	3.11212900	0.81272366	H	1.06462019	-0.10783266	2.26492848
H	-1.78182490	4.64641983	1.34115361	H	1.32214024	-1.83084320	1.92483982
H	-2.82411571	4.76426300	-0.95346116	H	1.84261030	-1.14539085	3.47875499
H	-1.12822857	5.20974720	-0.96140655	C	3.99297389	-1.87917989	2.07955545
H	-2.34112410	2.51640900	-1.78751431	H	3.84948503	-2.20903906	3.11907596
H	-1.55370462	3.68890449	-2.85216400	H	3.68941966	-2.71133586	1.42513285
N	-0.10947506	2.06627183	-0.18939179	H	5.06804493	-1.72663418	1.94589531
C	4.15189915	0.21084280	-0.33706620	C	5.25178626	-0.84405229	-0.57899118
C	3.13822124	-0.62420741	1.80623628	H	5.97019514	-0.47141567	-1.32404292
C	3.73659241	0.57830623	2.55363150	H	5.83094121	-1.09967246	0.31297906
C	4.99477237	1.11942346	1.88639484	H	4.82129783	-1.77774137	-0.97463583
C	4.74554067	1.41359574	0.41249958	C	3.72906461	0.66749072	-1.73239227
H	2.97642457	1.37955272	2.58223381	H	3.32320419	-0.17107422	-2.32506262
H	3.94436733	0.30263151	3.60141970	H	2.96106476	1.45103420	-1.68700753
H	5.33003080	2.03207813	2.40058984	H	4.58693216	1.07349755	-2.28750675
H	5.82173242	0.39855486	1.99428565	C	0.80731971	4.13190029	0.99296058
H	4.03275560	2.25409593	0.32942567	H	0.68142403	4.70644999	1.92253402
H	5.67832377	1.73960472	-0.07814069	H	1.77937018	3.61928383	1.04520652
N	2.94871160	-0.31279398	0.36367741	H	0.85346335	4.85705913	0.17548781
Cu	1.41030212	0.88744187	0.12483358	C	-0.41776080	2.42170544	2.22366519
Li	2.06836012	-1.71307757	-0.62123509	H	0.54952239	1.98703969	2.51636491
C	2.70650824	-3.87528567	-2.15949068	H	-0.70220305	3.14896985	2.99779433
C	2.16944570	-4.30812941	-0.94561984	H	-1.16970999	1.61878929	2.22908181
C	0.94037892	-3.80516089	-0.50297018	C	0.94794688	3.51293755	-2.02567265

H	1.06849769	3.47918446	-3.11850059	H	-4.18642223	1.41873660	-0.32022208
H	0.76323819	4.56095109	-1.76678484	H	-5.48611655	0.66561646	-1.27234561
H	1.90547590	3.22379366	-1.57334517	H	-5.43339751	0.44293220	0.47510981
C	-0.09923955	1.35711943	-2.53974706	C	-3.73614015	-0.10680583	2.49621770
H	0.91540088	0.93209313	-2.55021644	H	-4.79714246	0.02828456	2.26281689
H	-0.79040399	0.55383472	-2.24769170	H	-3.67592888	-0.35004702	3.56734756
H	-0.34389997	1.65930816	-3.56900434	H	-3.23827231	0.86079242	2.34191408
C	-3.42170490	-0.59730411	-2.10123368	C	-1.74593072	-1.53756444	2.37781508
H	-2.91766284	0.36387463	-2.27513311	H	-1.19110692	-2.33209105	1.85293154
H	-2.71960960	-1.40727441	-2.35899042	H	-1.09079330	-0.65690186	2.44313364
H	-4.26836201	-0.65485961	-2.80068237	H	-1.94221144	-1.88645870	3.40212361
C	-4.80713261	0.51624156	-0.41960451				

5-c)

Cartesian Coordinates

C	-4.00196000	0.51299500	0.68618400	C	-0.09879400	-2.58028200	1.71001700
C	-3.21919600	0.87771500	-1.69801000	C	1.07345000	-3.55375800	1.91047600
C	-4.14794000	2.09789400	-1.79295800	C	1.05028400	-4.72082900	0.93308900
C	-5.36217600	1.99477300	-0.88478000	C	0.95536700	-4.22390700	-0.50242600
C	-4.91813300	1.73903700	0.54604800	H	2.01783700	-2.99673000	1.77904200
H	-3.56689100	2.99310800	-1.50900000	H	1.06771400	-3.92224500	2.94978600
H	-4.45633600	2.23773700	-2.84218300	H	1.95469300	-5.33375000	1.05949000
H	-5.95294400	2.92097900	-0.93690000	H	0.20456500	-5.39024300	1.15908000
H	-6.03404600	1.19199500	-1.22965600	H	1.89173500	-3.69903800	-0.76514900
H	-4.36515300	2.62264000	0.91060600	H	0.86595200	-5.07421200	-1.19851800
H	-5.79113900	1.61447000	1.20775400	N	-0.16785600	-2.14962000	0.27801100
N	-2.86306100	0.60114900	-0.27589600	C	3.00831800	0.63590800	-1.87823500
Cu	-1.45725400	1.80377100	0.37862600	C	4.05914100	-0.01697500	0.31664000
Cu	-1.49979300	-0.76964500	-0.02968700	C	5.08235800	1.12033700	0.13910400
C	-0.21576100	-3.25511000	-0.72839700	C	5.34756100	1.47210000	-1.31486900

C	4.03434200	1.77390900	-2.01747500
H	4.69342500	2.01948100	0.65403300
H	6.01999600	0.85062700	0.65245500
H	6.02236000	2.33839200	-1.37891200
H	5.87316100	0.64564100	-1.81960500
H	3.59973100	2.69258100	-1.57966500
H	4.20153400	1.98747600	-3.08615000
N	2.82180900	0.27375400	-0.44988900
Cu	1.33715200	-0.93901100	-0.12774600
Li	1.80136300	1.67508000	0.43863000
C	2.39835600	4.15729100	1.93530100
C	1.85911000	4.45340300	0.68259500
C	0.68253500	3.82565700	0.25987200
C	-0.00881100	2.87538800	1.04694600
C	0.56029000	2.62894600	2.31832200
C	1.73305100	3.24995000	2.76067700
H	3.32424200	4.62801400	2.26401200
H	2.36310700	5.16598200	0.02816900
H	0.30017400	4.07543700	-0.73390000
H	0.08360000	1.90485800	2.98569200
H	2.13862200	3.01206900	3.74511700
C	3.70910700	-0.07145400	1.80453800
H	3.16515100	0.82710400	2.14351200
H	3.09802000	-0.95234400	2.04562000
H	4.62456300	-0.13220500	2.41098200
C	4.72009000	-1.36802900	-0.00899500
H	5.48761800	-1.61141100	0.74183600
H	3.96723100	-2.17029400	0.00338700
H	5.21075400	-1.38907200	-0.98768100
C	3.41875800	-0.52545400	-2.80438600
H	3.24172800	-0.25597600	-3.85672500
H	4.47734600	-0.79468700	-2.72062200
H	2.83288400	-1.42857800	-2.58336400

C	1.67057900	1.15465100	-2.40297100
H	0.90581900	0.36470000	-2.39475300
H	1.28543400	1.99757500	-1.80469200
H	1.76823000	1.51654200	-3.43688400
C	-1.39030000	-3.21955100	2.25400600
H	-1.53289200	-4.26088900	1.94923600
H	-1.36968300	-3.21402900	3.35378700
H	-2.27520700	-2.65263000	1.93265400
C	0.14089400	-1.34349700	2.57641200
H	-0.72325400	-0.66321000	2.55257900
H	0.31038000	-1.63773100	3.62258000
H	1.01838100	-0.77340300	2.24169400
C	-1.54385100	-4.03155700	-0.75750800
H	-1.59781600	-4.63888000	-1.67300100
H	-1.67797800	-4.71720700	0.08424200
H	-2.39673700	-3.33682900	-0.76479800
C	-0.06781400	-2.64651900	-2.12105700
H	-0.92310600	-1.99890700	-2.36858700
H	0.84920400	-2.04549500	-2.20518800
H	-0.01764000	-3.43870200	-2.88190000
C	-3.44644300	0.51725200	2.11081300
H	-2.86877400	-0.39500000	2.32047500
H	-2.79457200	1.38742900	2.29230200
H	-4.27040900	0.55982500	2.83790300
C	-4.83036500	-0.77764900	0.56052100
H	-5.46430300	-0.90598000	1.45046000
H	-5.49762600	-0.79120900	-0.30728300
H	-4.16907700	-1.65348000	0.48689000
C	-3.85148300	-0.31936100	-2.42894900
H	-4.88390400	-0.52383600	-2.12852000
H	-3.86601500	-0.13349700	-3.51319500
H	-3.26620700	-1.23340600	-2.25086400
C	-1.93987300	1.21027500	-2.46236600

H -1.40852700 2.06429800 -2.01190400
H -1.25015200 0.35345700 -2.47570700

H -2.17234900 1.47085500 -3.50519700

5-d)

Cartesian Coordinates

C 4.02606100 -0.26050400 0.61993400
C 3.24624300 -0.70206100 -1.75283300
C 4.29017500 -1.82456600 -1.86002600
C 5.50361600 -1.59731800 -0.97508500
C 5.05661100 -1.38994500 0.46192100
H 3.80615900 -2.77134000 -1.56171700
H 4.59078700 -1.93879400 -2.91452300
H 6.18568600 -2.45775900 -1.03857300
H 6.08269700 -0.72924500 -1.32985600
H 4.59935200 -2.32526000 0.83005000
H 5.92131600 -1.18058800 1.11310800
N 2.88539100 -0.45327200 -0.32650000
Cu 1.58968000 -1.75366200 0.36139400
Cu 1.40812300 0.80059800 -0.05708100
C -0.05707900 3.21234600 -0.66570100
C -0.00952300 2.49554600 1.76253700
C -1.15917500 3.47309900 2.05602100
C -1.19464800 4.65737400 1.10254000
C -1.21499100 4.16710200 -0.33611300
H -2.11569200 2.93033500 1.97789000
H -1.07977000 3.81716700 3.10054800
H -2.08197400 5.27520600 1.30383700
H -0.32823600 5.31707500 1.27069900
H -2.16373400 3.62970600 -0.51536400
H -1.19592500 5.01750700 -1.03734200

N -0.01177200 2.08654000 0.31977800
C -4.12097000 -0.23561400 0.25938900
C -2.91114500 -0.99547400 -1.80835200
C -3.68639900 0.04208000 -2.63534100
C -5.04170700 0.38383300 -2.03296200
C -4.88211800 0.80320800 -0.57888400
H -3.08198700 0.96433200 -2.68983200
H -3.80154200 -0.32008000 -3.67085000
H -5.51763400 1.19098700 -2.60889600
H -5.72474600 -0.47798300 -2.10955600
H -4.31466400 1.75070300 -0.54212100
H -5.86605000 1.00354800 -0.12224100
N -2.82491600 -0.59717900 -0.37475100
Cu -1.42344500 0.75125800 -0.06033600
Li -1.81889400 -1.91952500 0.61261400
C -2.13730100 -4.20580400 2.06674800
C -1.60066400 -4.53726700 0.82128300
C -0.45627200 -3.88186100 0.35255400
C 0.21014700 -2.87512900 1.08852700
C -0.34935000 -2.59880800 2.35920200
C -1.49597000 -3.23787500 2.84345200
H -3.04158000 -4.69472100 2.42729800
H -2.08719800 -5.29428000 0.20465100
H -0.08564100 -4.15227200 -0.64006700
H 0.10943400 -1.83152200 2.98925400

H	-1.89875900	-2.97114800	3.82149200	C	1.25899900	4.00134900	-0.77691900
C	-1.49015000	-1.08762700	-2.35676600	H	1.21632500	4.67944200	-1.64200200
H	-0.96110600	-0.12947600	-2.26673400	H	1.48348500	4.61669600	0.09867700
H	-0.89776900	-1.84503700	-1.81700700	H	2.10692700	3.31686500	-0.92838000
H	-1.49412500	-1.36882800	-3.42029400	C	-0.31413400	2.63689600	-2.05560300
C	-3.52660400	-2.39216500	-2.04202900	H	0.48352900	1.94034200	-2.35729200
H	-3.29768500	-2.73529900	-3.06172200	H	-1.27356900	2.10024000	-2.09655200
H	-3.10563500	-3.13481700	-1.34568700	H	-0.35397600	3.44288800	-2.80230700
H	-4.61541800	-2.42320700	-1.93893300	C	3.49786900	-0.32965500	2.05359400
C	-5.03622600	-1.44494000	0.54464400	H	2.82715900	0.51120900	2.28106900
H	-5.85196400	-1.14877200	1.22064100	H	2.94872500	-1.26715500	2.23928000
H	-5.50618800	-1.87111800	-0.34628100	H	4.33419300	-0.28598800	2.76644700
H	-4.47565800	-2.25303300	1.04235800	C	4.72569000	1.10374700	0.48670000
C	-3.83608800	0.37808600	1.62723600	H	3.98480800	1.91294500	0.41149800
H	-3.29698200	-0.32731800	2.28235800	H	5.34878000	1.29640100	1.37272600
H	-3.23074800	1.29050600	1.53667100	H	5.38510200	1.17612700	-0.38458100
H	-4.77240100	0.64854000	2.13637200	C	3.74376700	0.54805600	-2.49770000
C	1.30960600	3.12959800	2.24819500	H	4.74063400	0.87803900	-2.18929800
H	2.18087700	2.59402600	1.84763700	H	3.79299600	0.34795000	-3.57844100
H	1.41674400	4.18491900	1.97713000	H	3.05226400	1.38904300	-2.34243600
H	1.36235400	3.08185500	3.34591900	C	1.99685300	-1.16623000	-2.49595500
C	-0.21367300	1.24440500	2.61703100	H	1.56723200	-2.07050000	-2.03507700
H	0.61983800	0.53594900	2.49647200	H	1.22081300	-0.38710600	-2.49825400
H	-0.27771100	1.51415600	3.68131200	H	2.23824200	-1.40402000	-3.54222800
H	-1.13971100	0.71700000	2.34874700				

5-e)

Cartesian Coordinates

C	-2.93310300	1.41850300	-1.68580100	C	-4.95752200	0.09481200	-0.01046100
C	-3.91284100	1.03477300	0.61014500	C	-5.26843300	0.42411100	-1.46270700

C	-3.98672900	0.47245000	-2.28136800	N	2.88662100	-0.05542500	-0.46619500
H	-4.56431000	-0.93648600	0.04590300	Cu	1.25252300	-1.05757800	-0.14938000
H	-5.87739900	0.11706500	0.59704300	Li	2.06369000	1.47175200	0.42156600
H	-5.95472300	-0.32665400	-1.88111900	C	3.02692800	3.84096800	1.85990000
H	-5.80220900	1.38591500	-1.53000700	C	2.45604000	4.19971900	0.63772200
H	-3.55649000	-0.54372300	-2.32813900	C	1.18280400	3.73154300	0.29611400
H	-4.20172300	0.77236900	-3.32043500	C	0.42283000	2.88382000	1.13614900
N	-2.69279800	1.08461500	-0.24915700	C	1.03301000	2.56477500	2.37086400
Cu	-1.17701100	2.03535600	0.50270400	C	2.30041700	3.03193800	2.73458300
Cu	-1.51232700	-0.49507500	0.00052800	H	4.02445800	4.18792200	2.12725700
C	-0.34640500	-2.48730300	1.73929800	H	3.00837600	4.83637200	-0.05482500
C	-0.66777000	-3.15688300	-0.68173800	H	0.77349000	4.02747200	-0.67429500
C	-1.97317800	-3.86575300	-0.28756100	H	0.50870500	1.90878600	3.07156200
C	-1.98110900	-4.35387900	1.15195500	H	2.73184100	2.74670200	3.69518500
C	-1.65729100	-3.20638000	2.09661300	C	3.69703400	-0.46980700	1.79888900
H	-2.80488600	-3.15132700	-0.42512200	H	3.40309600	0.55054300	2.09826500
H	-2.15702700	-4.70156600	-0.98243300	H	2.87864000	-1.15402300	2.06468500
H	-2.96430000	-4.77925300	1.40066200	H	4.56504500	-0.74019200	2.41766600
H	-1.25976700	-5.17688500	1.28054400	C	4.42891800	-2.02190900	0.04245000
H	-2.48462200	-2.47770900	2.06245200	H	4.90688800	-2.17422900	-0.93140700
H	-1.59863400	-3.56551900	3.13741200	H	5.13384300	-2.38452400	0.80635200
N	-0.34960000	-2.07067900	0.29819500	H	3.53547500	-2.66240800	0.07560700
C	3.12668400	0.23924400	-1.90130900	C	3.24325900	-1.00119800	-2.80498800
C	4.04879600	-0.55472000	0.31243000	H	3.21124300	-0.70938700	-3.86596000
C	5.28063600	0.34072500	0.09035300	H	4.17140100	-1.56300100	-2.65465700
C	5.59971400	0.56368700	-1.37787100	H	2.40679500	-1.69123300	-2.61940800
C	4.37394800	1.12128600	-2.08050700	C	1.92767000	1.03331600	-2.41479100
H	5.08692800	1.32263500	0.56136600	H	1.00201300	0.44420500	-2.34515300
H	6.14518300	-0.09371300	0.61864200	H	1.77696000	1.96748000	-1.84671200
H	6.44784300	1.25619100	-1.48235600	H	2.06510600	1.32091800	-3.46733000
H	5.92086900	-0.37835700	-1.85082500	C	0.46041900	-4.18639000	-0.86448400
H	4.15526100	2.12275800	-1.66497700	H	0.62457900	-4.82753300	0.00592000
H	4.56736000	1.26505100	-3.15617400	H	0.22715100	-4.84912800	-1.71083100

H	1.41036500	-3.67886200	-1.08955000	H	-1.19427800	0.24041600	-2.29447000
C	-0.88260100	-2.53209900	-2.05711500	H	-1.79159500	1.36571500	-3.53135100
H	0.01109000	-1.98626100	-2.39742700	C	-3.34382400	2.88207100	-1.94221800
H	-1.10206400	-3.31115500	-2.80115600	H	-2.71544500	3.56698400	-1.35429200
H	-1.73128400	-1.83306300	-2.05169800	H	-3.20105100	3.12255700	-3.00620500
C	0.83544300	-3.39100200	2.14757200	H	-4.39021000	3.10215000	-1.71151600
H	0.97396000	-3.34745500	3.23802400	C	-4.53836500	2.41247000	0.89500700
H	0.69256300	-4.44675900	1.89492000	H	-5.06973200	2.84672300	0.04384000
H	1.77174900	-3.06052200	1.67767200	H	-5.26944400	2.32584300	1.71226900
C	-0.22622500	-1.23406000	2.60760900	H	-3.76345400	3.12652200	1.20936700
H	0.75676400	-0.75423400	2.48690200	C	-3.53301200	0.47590100	1.97712000
H	-0.98960200	-0.48503300	2.36064400	H	-3.10906900	-0.53380300	1.89230200
H	-0.34106200	-1.49567700	3.66971800	H	-2.79707200	1.12068300	2.48395100
C	-1.62581000	1.23782800	-2.45162500	H	-4.42064600	0.40842400	2.62217500
H	-0.87794000	1.98271900	-2.13614400				

5-f)

Cartesian Coordinates

C	-3.02025900	-1.18689000	1.73726100	Cu	-1.30309800	-2.03640600	-0.41386300
C	-3.95268200	-0.84894200	-0.58381300	Cu	-1.45316900	0.53602100	-0.01710800
C	-4.91358800	0.21356500	-0.02900300	C	-0.20445300	2.40952600	-1.81868300
C	-5.25367300	0.00164400	1.43913700	C	-0.42705600	3.15677500	0.58122900
C	-3.98478400	-0.11734000	2.27149500	C	-1.72251700	3.89748800	0.20974000
H	-4.43345400	1.20197600	-0.14646900	C	-1.77375100	4.33533900	-1.24485500
H	-5.83190500	0.23291700	-0.63906900	C	-1.50622000	3.15269800	-2.16360700
H	-5.86843900	0.83609700	1.80733600	H	-2.57156600	3.21893500	0.40890800
H	-5.87474800	-0.90072600	1.55931600	H	-1.84915700	4.76454700	0.87871000
H	-3.46307000	0.85624100	2.26736500	H	-2.75657100	4.77325900	-1.47260200
H	-4.23203600	-0.33878000	3.32308000	H	-1.04195300	5.13900200	-1.42549500
N	-2.74487300	-0.94888000	0.28824500	H	-2.35220800	2.44948100	-2.08953100

H -1.46374600 3.48193800 -3.21523500
N -0.18702300 2.02417800 -0.36871200
C 4.10368300 0.21501100 -0.33748700
C 3.11578200 -0.42565900 1.88032600
C 3.68654500 0.85737400 2.50444000
C 4.92586700 1.36623400 1.77826200
C 4.66720500 1.50272600 0.28262700
H 2.90416900 1.63615200 2.46470900
H 3.90894200 0.68837800 3.57170400
H 5.23399900 2.33581900 2.19625500
H 5.77486600 0.68554700 1.95491600
H 3.93380700 2.31233700 0.11670300
H 5.59134300 1.80018500 -0.24151100
N 2.91130300 -0.25854700 0.41625100
Cu 1.34659200 0.88944500 0.07064900
Li 2.06285500 -1.75918600 -0.43824400
C 2.79970900 -4.04467900 -1.78381900
C 2.22483800 -4.37897700 -0.55629100
C 0.97411400 -3.85878100 -0.20310900
C 0.23879300 -2.98744000 -1.04091200
C 0.84847600 -2.69947000 -2.28456600
C 2.09708700 -3.20994100 -2.65567600
H 3.78224200 -4.42787900 -2.05691600
H 2.75974700 -5.03234600 0.13423200
H 0.56750400 -4.12842300 0.77561400
H 0.34309400 -2.02753300 -2.98386100
H 2.53260300 -2.94193800 -3.61933100
C 1.75686400 -0.71720100 2.50967900
H 1.03225100 0.08088400 2.29680700
H 1.33421600 -1.65955900 2.12260700
H 1.83798500 -0.81478800 3.60217000
C 4.00113100 -1.62857400 2.26787600
H 3.86358800 -1.86376400 3.33358300

H 3.71889300 -2.52491600 1.69361500
H 5.07253100 -1.46342800 2.12065700
C 5.22960000 -0.83234700 -0.46774400
H 5.93245900 -0.52781100 -1.25718600
H 5.82186700 -0.96894600 0.44148300
H 4.82218100 -1.81585300 -0.75085300
C 3.67290100 0.50762000 -1.77338300
H 3.29961100 -0.40287500 -2.27448800
H 2.87874700 1.26358900 -1.81334400
H 4.51927900 0.88183800 -2.36711200
C 0.74230300 4.15168600 0.68020200
H 0.88347500 4.76663100 -0.21282600
H 0.57277300 4.84115800 1.52028800
H 1.68457000 3.61670800 0.87120900
C -0.61249900 2.60257100 1.99008500
H 0.28840700 2.07820800 2.34203900
H -0.81623600 3.42092900 2.69537600
H -1.46189200 1.90693900 2.04049300
C 0.98339200 3.28747200 -2.27416100
H 1.17711600 3.12452400 -3.34455000
H 0.80274500 4.36136900 -2.15347600
H 1.90248900 3.04522300 -1.72661700
C -0.13217100 1.13363400 -2.65966900
H 0.85305600 0.65140200 -2.57571800
H -0.88684200 0.39537700 -2.35738700
H -0.29659300 1.37043100 -3.72126800
C -1.70413100 -1.09124800 2.50295100
H -1.03271900 -1.92222800 2.23407700
H -1.17424100 -0.15349400 2.29430300
H -1.88439100 -1.14227300 3.58671500
C -3.56600700 -2.59092100 2.06551900
H -3.43451200 -2.79299100 3.13884400
H -4.63135400 -2.72081900 1.85414500

H	-3.01237200	-3.35984200	1.50751700	C	-3.52015300	-0.41232400	-1.97951100
C	-4.69417200	-2.18262000	-0.79027300	H	-3.00602300	0.55709100	-1.95463600
H	-5.27451100	-2.51165700	0.07590000	H	-2.84374200	-1.15095500	-2.43946500
H	-5.40317500	-2.08573500	-1.62557900	H	-4.39623100	-0.30508600	-2.63488500
H	-3.98174600	-2.98099200	-1.04331300				

5-g)

Cartesian Coordinates

C	3.12060800	-1.16142100	-1.68135000	H	0.08189500	5.32899900	1.28385400
C	3.95783900	-0.86913400	0.68573000	H	-1.60817400	3.75146400	-0.72989100
C	4.96257100	0.18069700	0.18773600	H	-0.51210300	5.09165700	-1.09065800
C	5.36297600	-0.02381400	-1.26655500	N	0.34939200	2.08336100	0.32597500
C	4.13121000	-0.10731900	-2.15732500	C	-3.02394900	-0.39319600	-1.91642300
H	4.49826300	1.17778800	0.29508800	C	-4.02277500	0.29224100	0.29459300
H	5.85327000	0.17459900	0.83775600	C	-5.15148800	-0.73185700	0.07470500
H	6.01194800	0.80008900	-1.59773300	C	-5.44243800	-1.00096300	-1.39143700
H	5.96854500	-0.93894100	-1.36865700	C	-4.16184300	-1.41290400	-2.09747800
H	3.62678800	0.87573400	-2.16454200	H	-4.85477000	-1.68328500	0.55572600
H	4.42245600	-0.32151800	-3.19907800	H	-6.05994300	-0.38974700	0.59718900
N	2.79098200	-0.93850300	-0.24298600	H	-6.20301300	-1.78944800	-1.49000100
Cu	1.29995500	-1.99303300	0.40973400	H	-5.87492600	-0.10639100	-1.86757400
Cu	1.55807700	0.58722000	0.00724500	H	-3.82882800	-2.38515000	-1.68777300
C	0.47521800	3.21336200	-0.64666400	H	-4.34061300	-1.57311200	-3.17353600
C	0.27950900	2.48982100	1.76626000	N	-2.81357800	-0.09033700	-0.47769500
C	-0.85829400	3.50295000	1.97191600	Cu	-1.23615900	0.99243600	-0.12212400
C	-0.77672800	4.68985200	1.02195800	Li	-1.90684600	-1.58476600	0.37834800
C	-0.65903700	4.22670800	-0.42289900	C	-2.75731800	-4.07750600	1.82414200
H	-1.82129800	2.98559800	1.81796700	C	-2.20415500	-4.38289000	0.57987700
H	-0.85192000	3.84892700	3.01909500	C	-0.97486300	-3.83026200	0.20535400
H	-1.66562800	5.32664500	1.14091600	C	-0.24220800	-2.94976800	1.03546400

C	-0.83171700	-2.68708800	2.29375000	H	0.82382700	0.54463200	2.60921000
C	-2.05661300	-3.23546800	2.68823700	H	-0.22137200	1.53560200	3.64979500
H	-3.72225500	-4.49036100	2.11629600	H	-0.90086500	0.70599100	2.23375900
H	-2.73709800	-5.04393600	-0.10494200	C	1.83676400	3.92916800	-0.61784700
H	-0.57962900	-4.08482200	-0.78237700	H	1.93817700	4.56312600	-1.51109300
H	-0.32669800	-2.01043600	2.98929700	H	1.98326500	4.57892600	0.24971400
H	-2.47455200	-2.99051600	3.66574500	H	2.65610700	3.19525200	-0.63300200
C	-3.67883000	0.25821700	1.78449900	C	0.34118900	2.66351400	-2.06467700
H	-3.23958100	-0.70641700	2.09198600	H	1.21015800	2.04850600	-2.34026500
H	-2.97666400	1.05727400	2.05972400	H	-0.56417100	2.05016400	-2.18243700
H	-4.58625600	0.39719100	2.39011800	H	0.27961800	3.49005400	-2.78728700
C	-4.54906300	1.71075700	0.01314600	C	1.84067900	-1.01093000	-2.49817400
H	-5.29886800	1.99922400	0.76592700	H	1.12185300	-1.81111700	-2.25974200
H	-3.72523700	2.43819200	0.06006200	H	1.34804900	-0.04767300	-2.30504100
H	-5.02412100	1.81235800	-0.96832900	H	2.06141100	-1.06607600	-3.57416300
C	-3.29993800	0.83138500	-2.80984300	C	3.64007300	-2.57449600	-2.00691200
H	-3.15233800	0.57417500	-3.86978800	H	3.02494500	-3.33515500	-1.50465900
H	-4.32201100	1.21467700	-2.71600300	H	3.57516400	-2.74964900	-3.09100800
H	-2.61709500	1.65656900	-2.56328200	H	4.68334200	-2.74480600	-1.72554200
C	-1.74405700	-1.03844400	-2.44497500	C	4.66572800	-2.21755000	0.91104400
H	-0.89271500	-0.34441700	-2.39446500	H	5.28515700	-2.54289000	0.07046800
H	-1.47157400	-1.94443400	-1.87663700	H	5.33191600	-2.14423200	1.78322200
H	-1.86371400	-1.34711500	-3.49370600	H	3.92898500	-3.00792900	1.11460900
C	1.58371900	3.08194500	2.33876200	C	3.46122600	-0.44004300	2.06373200
H	1.59197100	2.96948400	3.43283100	H	2.95067300	0.53168400	2.02364700
H	2.46785000	2.56561700	1.94237500	H	2.76091900	-1.18045800	2.48401000
H	1.70643800	4.15094900	2.13575000	H	4.30532200	-0.34211600	2.76136600
C	-0.02093400	1.24803800	2.60712500				

5-h)

Cartesian Coordinates

C	3.18746300	-0.93686800	-1.74021500	H	-5.31991600	1.72871300	-2.55785200
C	3.99065200	-0.66674500	0.63791400	H	-5.70049400	0.06775400	-2.14153400
C	4.90321700	0.48453700	0.18934600	H	-4.09193600	2.06544400	-0.45710800
C	5.32236800	0.37512000	-1.27016900	H	-5.71367000	1.45394400	-0.08557400
C	4.10583800	0.21624800	-2.17174500	N	-2.83795900	-0.41538500	-0.40348700
H	4.35585800	1.43310800	0.33510800	Cu	-1.33468700	0.80983700	-0.04232800
H	5.79040000	0.52723800	0.84282800	Li	-1.95721000	-1.84787300	0.53760400
H	5.89514200	1.26665500	-1.56490800	C	-2.50822800	-4.14893900	1.92093600
H	6.00853600	-0.47666000	-1.40524500	C	-1.97444000	-4.48490500	0.67545300
H	3.51687000	1.15097500	-2.15025400	C	-0.77093500	-3.91139000	0.24966900
H	4.41934800	0.06430800	-3.21801100	C	-0.04164600	-2.98482000	1.03018700
N	2.83362200	-0.79208100	-0.29806300	C	-0.60462700	-2.69957600	2.29729900
Cu	1.43232500	-1.96522400	0.34577200	C	-1.80813700	-3.25968200	2.73970900
Cu	1.47639600	0.62715600	-0.00415700	H	-3.45628500	-4.57358100	2.24901100
C	0.19794100	3.18760300	-0.58070500	H	-2.50770500	-5.18052700	0.02605700
C	0.17247100	2.42316700	1.82545600	H	-0.40107200	-4.18089000	-0.74340100
C	-0.93859100	3.44323200	2.12642400	H	-0.10070800	-1.98831200	2.95774700
C	-0.91196200	4.64713700	1.19842300	H	-2.20949800	-2.99058000	3.71767200
C	-0.92089200	4.18915200	-0.25019100	C	-1.54314800	-0.95699700	-2.39818000
H	-1.91699600	2.94522800	2.02843800	H	-0.91070700	-0.07164100	-2.25193300
H	-0.85465700	3.76187200	3.17880300	H	-1.04498000	-1.80481000	-1.89804600
H	-1.77940100	5.29367400	1.39641700	H	-1.56596900	-1.17755200	-3.47565200
H	-0.02536600	5.27088400	1.39569300	C	-3.69948900	-2.06198600	-2.14785100
H	-1.88914500	3.70136700	-0.46511100	H	-3.49192900	-2.38506000	-3.17860500
H	-0.84546700	5.05360100	-0.93003000	H	-3.36079100	-2.86869300	-1.47821500
N	0.16609500	2.03572500	0.37580300	H	-4.78733900	-1.99072900	-2.05596300
C	-4.10098900	0.03203400	0.24250500	C	-5.13133100	-1.09662400	0.45802000
C	-2.95223800	-0.74334200	-1.85247400	H	-5.91514900	-0.76144000	1.15323900
C	-3.61567100	0.40082900	-2.63501600	H	-5.64003200	-1.42046300	-0.45432500
C	-4.93390200	0.85053000	-2.01980100	H	-4.65477900	-1.98426600	0.90492500
C	-4.74876400	1.18103100	-0.54533100	C	-3.77222800	0.53889100	1.64385500
H	-2.92252800	1.25995000	-2.64994300	H	-3.31196700	-0.25162600	2.26132200
H	-3.76197200	0.09704900	-3.68529100	H	-3.07939700	1.39015900	1.60878100

H	-4.68267900	0.87188200	2.16259400	C	1.90508100	-0.86768400	-2.56177500
C	1.51059900	3.00825200	2.33057600	H	1.25547400	-1.73307000	-2.35699100
H	1.61262600	2.83102200	3.41128600	H	1.33140700	0.04224000	-2.33881800
H	2.37159100	2.54547400	1.83238200	H	2.13567600	-0.86521200	-3.63701100
H	1.59199200	4.09134200	2.18553100	C	3.82784800	-2.28816300	-2.11027900
C	-0.09667500	1.17025100	2.65976700	H	3.28410800	-3.11488100	-1.63107800
H	0.71370800	0.43377700	2.55899800	H	3.77381900	-2.43454000	-3.19918900
H	-0.18252500	1.43315400	3.72427600	H	4.88338300	-2.37439400	-1.83655500
H	-1.03268100	0.67847000	2.35941300	C	4.81123400	-1.95885300	0.80815500
C	1.55382800	3.91126700	-0.64290800	H	5.46956600	-2.18662900	-0.03478200
H	1.55854600	4.62140400	-1.48304700	H	5.45586100	-1.87133300	1.69508400
H	1.79789600	4.48061100	0.25811100	H	4.14432000	-2.81965500	0.95975700
H	2.36533600	3.18742500	-0.81107300	C	3.46058600	-0.34575000	2.03300300
C	-0.05805300	2.67766000	-1.99547000	H	2.85369800	0.56842300	2.03504400
H	0.74122300	2.00320400	-2.33513100	H	2.84152000	-1.17003900	2.42382600
H	-1.01687400	2.14347600	-2.06406100	H	4.29464700	-0.19148000	2.73261700
H	-0.09867700	3.52102300	-2.69966300				

Structure optimization for 7

7-a)

Cartesian Coordinates

C	4.01225100	-0.56508800	0.64861900	C	-5.65056800	-0.71173400	-1.46683200
C	3.20166500	-0.86244200	-1.71574700	C	-4.36392600	-1.16201000	-2.14214100
C	4.03253300	-2.15100400	-1.83079800	H	-5.22375800	-1.59358400	0.44166300
C	5.25619400	-2.14130000	-0.92739100	H	-6.34521200	-0.22710600	0.53387900
C	4.84555100	-1.85036900	0.50774300	H	-6.46002200	-1.42727200	-1.67373700
H	3.38721800	-3.00131700	-1.54612500	H	-5.98819600	0.24990000	-1.88681800
H	4.32644900	-2.31146800	-2.88202200	H	-4.12076900	-2.18274900	-1.79207800
H	5.77510500	-3.10959000	-0.98298100	H	-4.49734500	-1.22875600	-3.23513800
H	5.98597000	-1.39244400	-1.27673900	N	-3.02256300	-0.04661800	-0.35328000
H	4.23532600	-2.69285100	0.87960200	Li	-2.17933500	-1.57394000	0.47031600
H	5.73322900	-1.78934000	1.15972400	C	-2.57309800	-3.89219800	1.81373900
N	2.86791400	-0.55255900	-0.30038900	C	-2.03302900	-4.17580300	0.55733400
Cu	1.41868200	-1.69101700	0.33919700	C	-0.83788800	-3.56864500	0.15557200
C	0.12603600	2.54183400	1.64446900	C	-0.12746100	-2.65116900	0.96451200
C	0.38990800	3.35266600	-0.70995600	C	-0.70028900	-2.41504300	2.23585400
C	1.69977300	4.06084300	-0.31273200	C	-1.88988300	-3.01685300	2.66036200
C	1.73639900	4.44914600	1.15890300	H	-3.51146700	-4.34747400	2.12851700
C	1.44221400	3.23856700	2.03485300	H	-2.55055700	-4.86158700	-0.11480800
H	2.54483800	3.37302700	-0.51467900	H	-0.45524200	-3.80960200	-0.83996200
H	1.86673700	4.94376600	-0.95255400	H	-0.21030000	-1.71813600	2.92191100
H	2.71903300	4.87243000	1.41441400	H	-2.29569700	-2.78752200	3.64667000
H	1.00580200	5.24990100	1.35835000	C	-3.94883400	0.14758700	1.87839700
H	2.27291500	2.51438700	1.92649600	H	-3.67437700	-0.89262200	2.12319300
H	1.42260600	3.52416100	3.10032700	H	-3.12729700	0.80403900	2.20823200
N	0.08501700	2.23540800	0.20149800	H	-4.82880100	0.39230800	2.49103500
C	-3.17542600	-0.24371500	-1.80945700	C	-4.66945400	1.80225900	0.22282000
C	-4.24280300	0.32771400	0.38705600	H	-5.44608800	2.07170800	0.95535600
C	-5.43030700	-0.58625100	0.03310800	H	-3.81388900	2.47756400	0.39277100

H	-5.07313200	2.03094400	-0.76946300	H	-0.95111000	0.73639700	2.24492800
C	-3.30725100	1.05828100	-2.63126300	H	0.78595900	0.47488700	2.03127800
H	-3.21094100	0.85322500	-3.70867400	H	0.18794000	1.33015000	3.46782400
H	-4.26400100	1.57096900	-2.48618100	C	3.46910900	-0.52717700	2.07851800
H	-2.51263800	1.77809400	-2.37035000	H	2.94298200	0.41730100	2.28660400
C	-1.89773100	-0.92182900	-2.30797500	H	2.77236500	-1.35804800	2.27726900
H	-1.00483500	-0.31132900	-2.08857200	H	4.29305700	-0.60455500	2.80298100
H	-1.74509400	-1.90824500	-1.84050000	C	4.92851200	0.66826200	0.53018500
H	-1.92162100	-1.08246800	-3.39578400	H	5.60579500	0.72419300	1.39565000
C	-0.73350900	4.39993900	-0.85791500	H	5.55780100	0.66852600	-0.36541700
H	-0.87121400	5.02001100	0.03442300	H	4.33047700	1.59351900	0.51628500
H	-0.52508500	5.08369500	-1.69556300	C	3.93101200	0.27905000	-2.45389800
H	-1.69657700	3.90639200	-1.06611500	H	4.98917000	0.36859400	-2.18784300
C	0.58507800	2.75373800	-2.10440700	H	3.89154500	0.11627300	-3.54132100
H	-0.32259600	2.22827000	-2.44576900	H	3.45884200	1.25122700	-2.24562000
H	0.81850300	3.52882200	-2.84876100	C	1.89388000	-1.08114600	-2.47907000
H	1.41730000	2.03082800	-2.13330400	H	1.30315700	-1.90565900	-2.04834400
C	-1.05551000	3.38115500	2.18048000	H	1.26375300	-0.17621800	-2.47261600
H	-1.10058500	3.32990900	3.27970400	H	2.09383700	-1.32724300	-3.53224000
H	-0.99723200	4.44197200	1.91380500	Li	1.54100400	0.92239000	-0.11632500
H	-2.01487600	2.99974800	1.79413300	Li	-1.55965700	1.26154300	-0.16222400
C	0.03892400	1.20372500	2.38476900				

7-b)

Cartesian Coordinates

C	-3.96485400	-0.51555600	-0.64210500	H	-3.51244400	-2.88695000	1.65018900
C	-3.17519200	-0.76290800	1.73948900	H	-4.39427200	-2.08276400	2.96078700
C	-4.09532200	-1.98346900	1.90360600	H	-5.90804800	-2.84610400	1.10119100
C	-5.31726100	-1.92363000	1.00146700	H	-5.98714500	-1.10533800	1.31298200
C	-4.88210900	-1.73419200	-0.44251300	H	-4.32754000	-2.63339300	-0.76524700

H	-5.75947200	-1.64713700	-1.10524700	C	1.85798100	-3.12985300	-2.61711800
N	-2.82508400	-0.52366000	0.31404200	H	3.44526500	-4.50645100	-2.09519000
Cu	-1.40148600	-1.70753600	-0.28814400	H	2.49107100	-4.98537000	0.15833700
C	-0.11631700	2.50086900	-1.71527300	H	0.44190700	-3.86176200	0.90632600
C	-0.28747800	3.35316200	0.62348600	H	0.20722400	-1.79337300	-2.87033000
C	-1.66573400	3.96471200	0.29864700	H	2.26236300	-2.91359900	-3.60684100
C	-1.83333800	4.30244400	-1.17665500	C	1.69272600	-0.54018200	2.28993500
C	-1.49776600	3.09757000	-2.04582700	H	1.09792000	0.36177800	2.07053600
H	-2.45111100	3.23674000	0.58617000	H	1.16786000	-1.39941400	1.83930900
H	-1.84391400	4.85715600	0.92200100	H	1.66583100	-0.67174700	3.38191300
H	-2.86352100	4.63534900	-1.37364600	C	3.83822800	-1.71709800	2.22529500
H	-1.18838300	5.15506200	-1.44362800	H	3.68334000	-1.88700400	3.30213000
H	-2.27097300	2.32108200	-1.88735300	H	3.43302200	-2.59499200	1.69497300
H	-1.55338600	3.36284900	-3.11547100	H	4.92027600	-1.70331000	2.05622800
N	0.01696300	2.22179900	-0.27123100	C	5.32508200	-0.95521300	-0.55113700
C	4.27631100	0.16591100	-0.38076000	H	6.11987300	-0.64539000	-1.24742200
C	3.12663500	-0.42488500	1.76771800	H	5.81524000	-1.24110700	0.38558800
C	3.79189000	0.78429800	2.44898100	H	4.85997700	-1.86408600	-0.96884700
C	5.11959600	1.15812200	1.80570100	C	3.88950900	0.58525300	-1.79966900
C	4.93426200	1.37313400	0.31033900	H	3.42656500	-0.25010200	-2.35322100
H	3.10767400	1.65077200	2.36763700	H	3.17392100	1.42267200	-1.79656800
H	3.91989000	0.59087000	3.52742800	H	4.76612900	0.91525500	-2.37602100
H	5.52534200	2.06737600	2.27310400	C	0.77373200	4.47180000	0.65381000
H	5.86758200	0.36924100	1.98846800	H	0.79779100	5.07777200	-0.25804500
H	4.28283500	2.25509800	0.15884900	H	0.58856400	5.16064100	1.49289500
H	5.89748700	1.61038600	-0.17214100	H	1.77656100	4.03857000	0.79060400
N	3.03692600	-0.24286200	0.30486400	C	-0.34451300	2.81107800	2.05253600
Li	2.25796600	-1.79211300	-0.50848200	H	0.64353600	2.45226500	2.38149900
C	2.52295900	-4.02403100	-1.77387400	H	-0.66537700	3.58845600	2.76135200
C	1.98568100	-4.28877300	-0.51180100	H	-1.05484500	1.97340300	2.15684700
C	0.81423300	-3.64309400	-0.09832700	C	0.96778500	3.41729500	-2.32740500
C	0.11902000	-2.71290500	-0.90630800	H	1.01208500	3.28632300	-3.41993800
C	0.68567800	-2.49903200	-2.18509600	H	0.79270900	4.48339800	-2.14507800

H	1.96076300	3.17685200	-1.91897400	H	-5.43361000	0.86074800	0.29859400
C	0.02343500	1.15777700	-2.44063200	C	-3.81528800	0.45482600	2.43596000
H	1.05856300	0.77998300	-2.38628000	H	-4.84762600	0.64567000	2.12591200
H	-0.62795400	0.37784000	-2.01172400	H	-3.83312400	0.30609000	3.52603900
H	-0.22876200	1.24800200	-3.50817100	H	-3.23917300	1.37224800	2.23795000
C	-3.41653400	-0.59397200	-2.06908100	C	-1.88658800	-1.05318100	2.51052000
H	-2.81454100	0.29050600	-2.32591800	H	-1.37324900	-1.94580800	2.11826500
H	-2.78929000	-1.48795500	-2.21835900	H	-1.17818700	-0.21021300	2.45899500
H	-4.24300200	-0.64440800	-2.79318500	H	-2.10157100	-1.23124500	3.57444200
C	-4.80409000	0.77674400	-0.59320400	Li	-1.47785100	0.93779000	0.10188500
H	-4.15434700	1.66635100	-0.62389800	Li	1.58614000	1.08984300	0.02682500
H	-5.47576700	0.82913300	-1.46327500				

7-c)

Cartesian Coordinates

C	4.09621700	-0.37066700	0.72665000	C	-1.16527600	3.53217100	1.88198400
C	3.35147100	-0.64547300	-1.66742500	C	-1.11936000	4.75588800	0.97652200
C	4.29747300	-1.84823800	-1.80995900	C	-0.98871900	4.33604800	-0.48154100
C	5.49781700	-1.76542600	-0.87881100	H	-2.10137900	2.97720800	1.67547300
C	5.03361600	-1.57728600	0.55782500	H	-1.21426300	3.83357800	2.94223100
H	3.72515800	-2.76170600	-1.56878400	H	-2.02486600	5.36464600	1.11620400
H	4.62414500	-1.94398600	-2.85924200	H	-0.27632400	5.40669100	1.26048000
H	6.10525200	-2.67848500	-0.96338300	H	-1.91734700	3.81377300	-0.78381700
H	6.16076900	-0.93752200	-1.17991300	H	-0.90721500	5.22155000	-1.13440400
H	4.48504300	-2.48200100	0.87480000	N	0.17380900	2.24961800	0.22010700
H	5.89797200	-1.47452800	1.23534700	C	-3.04170000	-0.44670600	-1.82964000
N	2.97868200	-0.41116700	-0.25017800	C	-4.17874900	0.06391900	0.33733800
Cu	1.55642500	-1.60352900	0.33689900	C	-5.17821600	-1.07949800	0.07144700
C	0.19983800	3.38589200	-0.71713900	C	-5.37371700	-1.36855200	-1.40952300
C	0.02714300	2.58572600	1.64882100	C	-4.02933200	-1.60024800	-2.08424000

H -4.79459000 -1.99631500 0.56104600
H -6.14488000 -0.85673800 0.55395200
H -6.02312600 -2.24650300 -1.54262100
H -5.90350400 -0.53156900 -1.89249000
H -3.58755100 -2.53520500 -1.68770400
H -4.15957200 -1.75646900 -3.16865900
N -2.90971600 -0.15155800 -0.38613700
Li -2.05477400 -1.68416800 0.45837900
C -2.32100800 -4.02585600 1.77675200
C -1.76254800 -4.27049600 0.52001100
C -0.60444500 -3.59228200 0.12399400
C 0.05130600 -2.64027600 0.93972600
C -0.53713600 -2.44536900 2.21103600
C -1.69193500 -3.11634300 2.62917700
H -3.23182500 -4.53676800 2.08693600
H -2.23773600 -4.98158200 -0.15710700
H -0.20772200 -3.80490400 -0.87260100
H -0.08989700 -1.72563400 2.90271800
H -2.11224700 -2.91634800 3.61578400
C -3.87548400 0.06542200 1.83815500
H -3.35494500 -0.85037500 2.16819900
H -3.25148700 0.92668100 2.12087900
H -4.80351700 0.12712900 2.42521700
C -4.86307500 1.41844700 0.06166000
H -5.67424600 1.59946400 0.78407900
H -4.13689800 2.24032100 0.16416600
H -5.30322400 1.49130400 -0.93827000
C -3.44669200 0.75144300 -2.71783400
H -3.21851900 0.54512600 -3.77495700
H -4.51417200 0.99181100 -2.66626200
H -2.89769700 1.66146400 -2.43076200
C -1.66171000 -0.88589600 -2.32597300
H -0.91997300 -0.07375600 -2.23686800

H -1.27050600 -1.74999100 -1.76517700
H -1.68877500 -1.17455200 -3.38692200
C 1.28061200 3.18764400 2.32173500
H 1.47424000 4.22688100 2.03517200
H 1.17945700 3.17176800 3.41815800
H 2.18135400 2.60571500 2.06739000
C -0.24188600 1.27126900 2.38737400
H 0.60607900 0.57328500 2.28111500
H -0.40547300 1.43668900 3.46282900
H -1.13625500 0.75255800 2.00658500
C 1.51102000 4.20170500 -0.72072500
H 1.54662700 4.88138800 -1.58634800
H 1.64576900 4.81791400 0.17472800
H 2.38461200 3.53266900 -0.79266400
C 0.07625000 2.80638400 -2.12725800
H 0.92873800 2.14633500 -2.36421800
H -0.84602700 2.21601500 -2.25138600
H 0.05408900 3.59829000 -2.89003500
C 3.50531200 -0.42925700 2.13699600
H 2.86235400 0.44291800 2.34118200
H 2.90259600 -1.33881400 2.29125500
H 4.30468300 -0.42644700 2.89245000
C 4.91698400 0.93361800 0.67815900
H 4.25353500 1.81339200 0.66888800
H 5.55932200 1.01442800 1.56781500
H 5.57442400 1.00957800 -0.19402300
C 3.97044600 0.58659600 -2.35704100
H 4.98581600 0.81746200 -2.01993200
H 4.02295800 0.43099700 -3.44506100
H 3.35382300 1.48366100 -2.18246500
C 2.07576200 -0.95497400 -2.45204200
H 1.56810300 -1.85330900 -2.06569600
H 1.35993800 -0.11700700 -2.40208100

H	2.30189600	-1.12744100	-3.51461300	Li	-1.41899300	1.12957500	-0.18361800
Li	1.67696200	1.04905900	-0.04492600				

7-d)

Cartesian Coordinates

C	4.11413500	-0.27982200	0.59840100	C	-4.15791700	-0.04479800	0.31482600
C	3.24525400	-0.51027900	-1.75718100	C	-3.02281700	-0.91059700	-1.74824000
C	4.17340800	-1.71692900	-1.96897900	C	-3.86067900	0.05648400	-2.60199300
C	5.42287100	-1.65505100	-1.10467100	C	-5.20347300	0.38123800	-1.96698400
C	5.03516100	-1.48768300	0.35653100	C	-4.98209600	0.91509500	-0.56081100
H	3.60882500	-2.63001800	-1.70861100	H	-3.29389700	0.99718800	-2.72120900
H	4.43975100	-1.79981400	-3.03619700	H	-3.99427600	-0.35801500	-3.61541200
H	6.01918900	-2.57004900	-1.23522600	H	-5.74375400	1.12154900	-2.57526700
H	6.07362300	-0.82643400	-1.42927400	H	-5.84694000	-0.51385700	-1.94324000
H	4.50118300	-2.39637900	0.68706900	H	-4.43296700	1.87183400	-0.63299100
H	5.93413900	-1.39885300	0.98952500	H	-5.94375000	1.14028000	-0.06965800
N	2.94423400	-0.29402300	-0.31886000	N	-2.90544500	-0.46423600	-0.34282100
Cu	1.56689300	-1.50602400	0.33868200	Li	-2.10426000	-1.94611500	0.60087700
C	-0.15329400	3.35207800	-0.68662400	C	-2.09595000	-4.10242100	2.03324300
C	0.16144300	2.56734200	1.66880100	C	-1.53221000	-4.40210000	0.79091200
C	-0.87736600	3.59608000	2.14876100	C	-0.44586500	-3.65849200	0.31477700
C	-0.94769000	4.81622500	1.24256100	C	0.13816800	-2.59304400	1.03903900
C	-1.19171500	4.37566300	-0.19244900	C	-0.44642600	-2.34876000	2.30446600
H	-1.86940700	3.11170800	2.16215800	C	-1.53765700	-3.07358500	2.79661900
H	-0.65990100	3.89237200	3.18906500	H	-2.95499100	-4.66213600	2.40120600
H	-1.75068000	5.49048500	1.57523000	H	-1.95280900	-5.20429100	0.18308100
H	-0.01758800	5.40406800	1.31113600	H	-0.05357800	-3.91031600	-0.67448700
H	-2.19052100	3.90469300	-0.24771300	H	-0.04968600	-1.54512100	2.93075600
H	-1.21673000	5.24572400	-0.87019000	H	-1.96160500	-2.82840700	3.77127300
N	-0.00781900	2.21815600	0.24345600	C	-1.60735900	-0.94428500	-2.32511800

H	-1.15265000	0.05840600	-2.32989200	H	1.57603900	4.64477600	-0.16738300
H	-0.95033500	-1.60939000	-1.73989200	H	1.94085000	3.36547500	-1.33684800
H	-1.59768700	-1.30237200	-3.36543100	C	-0.65624800	2.79079800	-2.01644600
C	-3.58690600	-2.33912500	-1.93221400	H	0.05198500	2.05306100	-2.43120300
H	-4.64769000	-2.42450200	-1.67263900	H	-1.63853600	2.30127100	-1.90366700
H	-3.48362800	-2.66740100	-2.97814100	H	-0.78236100	3.58344100	-2.76840200
H	-3.03753200	-3.07182000	-1.31634100	C	3.60528600	-0.37067000	2.03973600
C	-5.06346000	-1.20985000	0.77443800	H	2.98256300	0.49641400	2.30874200
H	-5.88328000	-0.84503900	1.41280700	H	3.00708000	-1.28138100	2.20553400
H	-5.52283600	-1.75772000	-0.05556900	H	4.45000400	-0.39713900	2.74374200
H	-4.49154300	-1.93942700	1.37460800	C	4.94405900	1.01817300	0.52871900
C	-3.77425100	0.70741900	1.58870000	H	4.29002200	1.90408000	0.52528200
H	-3.19360600	0.06613300	2.27355200	H	5.60465900	1.09706000	1.40497400
H	-3.17084200	1.60141400	1.36043500	H	5.58690000	1.08219200	-0.35563300
H	-4.66301200	1.05273400	2.13707400	C	3.83555800	0.72950700	-2.45681500
C	1.56531700	3.09482500	2.05362900	H	4.85294000	0.97509100	-2.13801100
H	1.74619100	4.12357300	1.72311400	H	3.86718900	0.57720000	-3.54611300
H	1.70286600	3.08058400	3.14608600	H	3.20978200	1.61791100	-2.26898700
H	2.37125100	2.47530200	1.62668700	C	1.93057100	-0.79980500	-2.48021800
C	-0.04147600	1.27587200	2.46426500	H	1.44416100	-1.70735300	-2.08917800
H	0.66406300	0.49110300	2.13898400	H	1.21661500	0.03518500	-2.37132600
H	0.10751200	1.43146000	3.54337000	H	2.09711000	-0.94404400	-3.55791100
H	-1.06054400	0.87948700	2.33129100	Li	1.61155400	1.15619300	-0.13159800
C	1.16666700	4.08397200	-1.01448700	Li	-1.42156200	0.85442900	-0.07906800
H	1.03054100	4.79908600	-1.84075800				

7-e)

Cartesian Coordinates

C	3.11475900	-1.32186300	-1.62355200	C	5.12095300	0.12883300	-0.04903700
C	4.01307000	-0.68348500	0.64215000	C	5.48523000	-0.41424100	-1.42071300

C	4.23567300	-0.50062600	-2.28143400	Li	-2.21082600	-1.45000000	0.49869000
H	4.76561100	1.16925400	-0.16687100	C	-2.81124900	-3.71104400	1.91608900
H	6.00798100	0.17144800	0.60445600	C	-2.22169500	-4.06573000	0.70078800
H	6.23424800	0.23338700	-1.89980700	C	-0.97702600	-3.53355000	0.34561500
H	5.95868400	-1.40517500	-1.32884800	C	-0.26311500	-2.62644300	1.16408600
H	3.85888900	0.52261600	-2.46117100	C	-0.89024300	-2.31336200	2.39170400
H	4.47009700	-0.92684200	-3.27088900	C	-2.12988700	-2.84074900	2.76921200
N	2.83909700	-0.83673600	-0.24885800	H	-3.78712900	-4.10755800	2.19426500
Cu	1.35081200	-1.79437500	0.53433200	H	-2.73778600	-4.74832800	0.02437600
C	0.04959300	2.59595900	1.62645800	H	-0.55298100	-3.82977700	-0.61850300
C	0.64019200	3.29709000	-0.70352700	H	-0.40189400	-1.61754000	3.07903400
C	1.79428200	4.14649900	-0.13976800	H	-2.57567800	-2.55623900	3.72334900
C	1.53093900	4.63196100	1.27731300	C	-4.03586700	0.32061800	1.72118400
C	1.20630100	3.44818900	2.17665100	H	-3.76415300	-0.70460200	2.02559700
H	2.70810300	3.52325100	-0.12980800	H	-3.24624600	1.00013000	2.07913400
H	2.00308100	4.99584400	-0.81204300	H	-4.95809400	0.57152600	2.26521100
H	2.40781500	5.17278000	1.66266000	C	-4.70719200	1.88426200	-0.04839300
H	0.70408000	5.36095800	1.28498200	H	-5.08077500	2.04524700	-1.06577200
H	2.10384500	2.81077300	2.25892600	H	-5.52375100	2.15766900	0.63771900
H	0.97032300	3.78780300	3.19944300	H	-3.88664600	2.60065700	0.11606500
N	0.25974300	2.20790300	0.21578000	C	-3.11336400	1.08860000	-2.76724900
C	-3.00725600	-0.17835100	-1.89033200	H	-2.95591700	0.84437700	-3.82924700
C	-4.23555100	0.43658100	0.20732300	H	-4.08278100	1.59213400	-2.69259500
C	-5.36625100	-0.53228900	-0.18748900	H	-2.34147400	1.82762600	-2.49069300
C	-5.48406900	-0.71663700	-1.69292400	C	-1.67940400	-0.83208500	-2.27242100
C	-4.14257300	-1.14541400	-2.26791300	H	-0.82516700	-0.17732100	-2.02743700
H	-5.15549500	-1.51742700	0.27043300	H	-1.52277000	-1.78846700	-1.74649200
H	-6.32330900	-0.18858700	0.24001900	H	-1.62168700	-1.04407500	-3.35047200
H	-6.25545900	-1.46555200	-1.92551200	C	-0.52080400	4.22634000	-1.11885800
H	-5.82280700	0.21822500	-2.16862100	H	-0.88729400	4.85672200	-0.30149200
H	-3.89182900	-2.14668800	-1.86961500	H	-0.21679600	4.90056000	-1.93463000
H	-4.20160000	-1.25144800	-3.36429300	H	-1.37735000	3.63726100	-1.48867200
N	-2.95672100	0.07578000	-0.43577000	C	1.13390400	2.64881500	-1.99834600

H	0.35902500	1.99977800	-2.44064000	C	3.45170300	-2.82286900	-1.72808700
H	1.40153400	3.40377900	-2.75172800	H	2.70747300	-3.42102700	-1.17938100
H	2.04171700	2.04120600	-1.83633500	H	3.43537100	-3.14587300	-2.78068600
C	-1.27306900	3.34802000	1.91181000	H	4.43907400	-3.08024300	-1.33070800
H	-1.47885800	3.37768400	2.99320800	C	4.59744100	-2.00311200	1.18155400
H	-1.26977800	4.38498300	1.55916900	H	5.12257400	-2.59103100	0.42145400
H	-2.13737000	2.85163000	1.43998700	H	5.32067500	-1.80266900	1.98725200
C	-0.02646600	1.30211900	2.44006100	H	3.79554700	-2.63325700	1.59473900
H	-0.87201700	0.67036400	2.11519000	C	3.56637500	0.10763300	1.86984600
H	0.88852900	0.69993200	2.33599300	H	3.16050700	1.09461300	1.59121000
H	-0.16773200	1.50635900	3.51204300	H	2.79856600	-0.43906800	2.44102500
C	1.84675900	-1.12574400	-2.45265300	H	4.41207400	0.29595600	2.54685300
H	1.02501700	-1.75786500	-2.07960500	Li	1.57807200	0.74475600	-0.06285300
H	1.50978100	-0.07809600	-2.43648300	Li	-1.46346200	1.35070400	-0.21177800
H	2.02012200	-1.39343900	-3.50548000				

7-f)

Cartesian Coordinates

C	-3.17902900	-1.11814700	1.63498400	Cu	-1.42935300	-1.73846900	-0.49343600
C	-4.02708900	-0.49475400	-0.65413500	C	0.12428800	2.53529100	-1.69302600
C	-5.09980600	0.38767700	0.00596300	C	-0.39376600	3.29479100	0.62478600
C	-5.49973100	-0.09981900	1.38849400	C	-1.52960700	4.17508100	0.06688200
C	-4.26222300	-0.22524900	2.26179900	C	-1.29066500	4.62178400	-1.36648800
H	-4.69574400	1.41263700	0.09936000	C	-1.01226100	3.41306000	-2.24780100
H	-5.97897900	0.45529200	-0.65593000	H	-2.46636400	3.58624600	0.09627000
H	-6.21873500	0.59692100	1.84412300	H	-1.69066800	5.04594500	0.72461000
H	-6.02185000	-1.06786600	1.31917600	H	-2.16453600	5.17356700	-1.74329000
H	-3.83577300	0.78241800	2.41778100	H	-0.44986400	5.33320100	-1.40789200
H	-4.52487800	-0.61283700	3.25999200	H	-1.92961100	2.80306600	-2.31507700
N	-2.86831000	-0.67967200	0.25145800	H	-0.77260400	3.72883100	-3.27767100

N	-0.08666500	2.16680800	-0.27647900	C	5.37752800	-0.97377200	-0.22333900
C	4.25714500	0.08973800	-0.25857700	H	6.18770500	-0.70464200	-0.91861600
C	3.00117400	-0.37404300	1.85333500	H	5.83581800	-1.10033200	0.76288500
C	3.53323900	0.93645000	2.46090600	H	4.98886700	-1.95741800	-0.53402700
C	4.87127500	1.35361800	1.86468700	C	3.96939900	0.31836300	-1.74360400
C	4.78940700	1.40239700	0.34421200	H	3.63621000	-0.61295000	-2.23429300
H	2.79369500	1.73860300	2.26667500	H	3.18783400	1.07427900	-1.90192400
H	3.60638400	0.84856500	3.55817400	H	4.86753800	0.66305100	-2.27658900
H	5.17195300	2.33518500	2.25964900	C	0.81702000	4.18092800	0.98326300
H	5.66029800	0.65146000	2.17992400	H	1.20094600	4.75665800	0.13464000
H	4.10621700	2.22324600	0.05317600	H	0.55794000	4.90243600	1.77387400
H	5.77315000	1.65162100	-0.08847100	H	1.64532300	3.55998900	1.36224700
N	2.98882000	-0.31251500	0.37822100	C	-0.88794700	2.71874900	1.95285800
Li	2.24374300	-1.86559400	-0.44377100	H	-0.12783600	2.07334900	2.42068800
C	2.56236500	-4.10479000	-1.67337100	H	-1.12634100	3.51886800	2.66850600
C	1.89187300	-4.35346500	-0.47297600	H	-1.81584800	2.13196800	1.83346900
C	0.70329000	-3.67389600	-0.18206600	C	1.46033800	3.26242800	-1.99574000
C	0.12206700	-2.72409100	-1.05604100	H	1.74315700	3.13838900	-3.05272200
C	0.82550000	-2.52043600	-2.26568100	H	1.41450700	4.34126800	-1.80711200
C	2.01515600	-3.18947700	-2.57639500	H	2.28955200	2.87391200	-1.38480500
H	3.49708500	-4.61545800	-1.90155300	C	0.15166400	1.23043700	-2.49514000
H	2.30431500	-5.06557100	0.24273200	H	1.00340600	0.58677300	-2.21262500
H	0.21870800	-3.88585500	0.77561700	H	-0.76516100	0.64036100	-2.34344600
H	0.44391000	-1.79647500	-2.99035400	H	0.24701100	1.42511900	-3.57376900
H	2.52658700	-2.98459100	-3.51785100	C	-1.91031700	-0.96840400	2.47283500
C	1.55111300	-0.56327800	2.30057000	H	-1.11989900	-1.65126700	2.12327100
H	0.88765800	0.24508300	1.95053700	H	-1.51539000	0.05774700	2.43715900
H	1.14003000	-1.51201700	1.91674000	H	-2.10832600	-1.20290700	3.52916600
H	1.45976800	-0.58287600	3.39685200	C	-3.59321700	-2.59743000	1.77168200
C	3.77068700	-1.56581000	2.46342800	H	-2.87937000	-3.24526500	1.23901800
H	3.52374900	-1.68024500	3.53032600	H	-3.59557500	-2.89687400	2.83132400
H	3.49415200	-2.50461100	1.95709000	H	-4.59158700	-2.81363800	1.37728900
H	4.85903700	-1.46574900	2.39879100	C	-4.67006700	-1.79865500	-1.16437100

H -5.22863700 -2.34068100 -0.39413000
H -5.37681200 -1.58469000 -1.98110800
H -3.89650700 -2.47705400 -1.55461200
C -3.53358800 0.24161800 -1.89768500
H -3.08989500 1.21784400 -1.64102900

H -2.78307800 -0.35155000 -2.44487500
H -4.36293400 0.44709000 -2.58972000
Li -1.54102200 0.84156900 0.04225500
Li 1.51172000 1.01879200 0.04622300

7-g)

Cartesian Coordinates

C 3.27324100 -0.82747100 -1.67810000
C 4.03421400 -0.92282200 0.72380200
C 5.23006000 -0.02748900 0.36367500
C 5.67329700 -0.19821000 -1.08072300
C 4.49541100 0.04616000 -2.00969600
H 4.93516800 1.02647900 0.52218300
H 6.06449500 -0.22957100 1.05536300
H 6.49020400 0.50034600 -1.31428500
H 6.08642400 -1.20742000 -1.23973400
H 4.19712300 1.10710400 -1.92071100
H 4.78564800 -0.10989800 -3.06184100
N 2.92498000 -0.72143000 -0.24110800
Cu 1.37349300 -1.75261400 0.27874300
C 0.29152100 3.41716200 -0.70234800
C 0.44736000 2.56931700 1.64286300
C -0.54301000 3.65297200 2.10558400
C -0.47761000 4.89974600 1.23663800
C -0.67341400 4.51990700 -0.22212400
H -1.56723300 3.23838600 2.05087700
H -0.36166200 3.90273600 3.16500300
H -1.24721800 5.62171100 1.54741500
H 0.48663900 5.41589300 1.37288400

H -1.70782000 4.14655700 -0.34586300
H -0.58495900 5.40644700 -0.87236500
N 0.30257500 2.25613900 0.20732300
C -3.16209200 -0.31034300 -1.82495300
C -4.11298700 0.36619900 0.38530100
C -5.15218300 -0.76908400 0.28308200
C -5.46287200 -1.16330000 -1.15437500
C -4.17932900 -1.46444700 -1.91738900
H -4.75528000 -1.65741000 0.81468000
H -6.07636000 -0.48768700 0.81569200
H -6.13008500 -2.03786600 -1.17151100
H -6.01967800 -0.35532400 -1.65552400
H -3.71908900 -2.38134200 -1.49721300
H -4.40091600 -1.69403200 -2.97349800
N -2.91164600 0.06766900 -0.41796900
Li -2.17370000 -1.55134600 0.38320200
C -2.64777000 -3.92068400 1.71297500
C -2.10159100 -4.20577100 0.45972000
C -0.90569300 -3.59843800 0.06208700
C -0.19877500 -2.68216900 0.87568800
C -0.77778600 -2.44299800 2.14360800
C -1.97126400 -3.04274800 2.56165200

H	-3.58787300	-4.37554100	2.02306200	H	-0.89593100	0.93645800	2.20089700
H	-2.61615000	-4.89201900	-0.21419000	C	1.68283900	4.02694600	-0.97010400
H	-0.51894600	-3.83656900	-0.93268700	H	1.63823300	4.78500900	-1.76774900
H	-0.29246800	-1.74345000	2.83052900	H	2.12105300	4.50925600	-0.08952600
H	-2.38365800	-2.81149800	3.54474800	H	2.38635900	3.24459300	-1.30073200
C	-3.67815500	0.46731500	1.84931200	C	-0.22678400	2.94174200	-2.06114600
H	-3.14410400	-0.43373400	2.19730700	H	0.40356400	2.14495400	-2.48271400
H	-3.01302600	1.33150300	2.00611200	H	-1.25896600	2.55867600	-1.99379300
H	-4.54550100	0.59949700	2.51256500	H	-0.25196600	3.76515400	-2.78975100
C	-4.79069900	1.71455900	0.06880700	C	2.09253300	-0.28181300	-2.48112000
H	-5.52188000	1.97578000	0.84973500	H	1.17580200	-0.86554100	-2.29701400
H	-4.03730000	2.51702400	0.03262900	H	1.89026500	0.77525100	-2.23913600
H	-5.32646200	1.72256000	-0.88604400	H	2.29775000	-0.31380200	-3.56075300
C	-3.63295900	0.82780600	-2.75620700	C	3.50139500	-2.26205700	-2.19051500
H	-3.50362100	0.53947100	-3.81083600	H	3.55733300	-2.27405700	-3.29012200
H	-4.68885500	1.08907400	-2.62841800	H	4.42532600	-2.71632500	-1.81842300
H	-3.04759200	1.74201600	-2.58554900	H	2.66596400	-2.91153200	-1.88620300
C	-1.82822800	-0.79083400	-2.40422200	C	4.51234400	-2.38151500	0.87054900
H	-1.09434400	0.03193800	-2.44617600	H	5.07388700	-2.74951300	0.00572200
H	-1.37818500	-1.60641000	-1.81317300	H	5.17374400	-2.47930400	1.74518500
H	-1.94973800	-1.16707000	-3.43050300	H	3.65362600	-3.05317600	1.02029800
C	1.86800800	3.00911100	2.07792200	C	3.53760300	-0.51076300	2.10942000
H	2.06867300	4.06773000	1.87613200	H	3.17878900	0.52804600	2.12140300
H	2.01546900	2.85747500	3.15849300	H	2.71592900	-1.16143100	2.45208800
H	2.65273400	2.43835900	1.55651400	H	4.34728600	-0.58359900	2.85010700
C	0.12847300	1.28293800	2.41074700	Li	1.71959200	0.88029700	-0.04573800
H	0.81276700	0.45926300	2.14331700	Li	-1.34360500	1.23638000	-0.17643300
H	0.20648000	1.42998400	3.49829000				

7-h)

Cartesian Coordinates

C	3.23516500	-0.54921100	-1.76186900	H	-3.26262800	1.16694500	-2.71657600
C	4.07407700	-0.73716800	0.60919200	H	-4.05782000	-0.13799400	-3.60517200
C	5.22636500	0.21777500	0.26050200	H	-5.69747000	1.42207400	-2.50734400
C	5.62958000	0.13722100	-1.20302000	H	-5.87363300	-0.21182400	-1.88749700
C	4.41454200	0.38586500	-2.08102200	H	-4.29918600	2.07942800	-0.59093700
H	4.90224500	1.25097100	0.48323700	H	-5.83487100	1.42810400	0.00170100
H	6.08819000	0.00940100	0.91579100	N	-2.90227200	-0.34590600	-0.36099600
H	6.41394000	0.87591000	-1.42432000	Li	-2.20188300	-1.90459400	0.52649300
H	6.07175800	-0.84688900	-1.42741600	C	-2.30539000	-4.10408500	1.94468800
H	4.08089100	1.42868900	-1.92467700	C	-1.76786100	-4.42253300	0.69554500
H	4.67567700	0.29795800	-3.14857200	C	-0.65677400	-3.72333500	0.20999900
N	2.92681800	-0.53182600	-0.31168400	C	-0.02395600	-2.68454200	0.93123300
Cu	1.44571800	-1.65326900	0.23684500	C	-0.58463700	-2.41891900	2.20327800
C	-0.08575700	3.35068000	-0.58564600	C	-1.69868200	-3.10121900	2.70518900
C	0.36655300	2.50462200	1.72074300	H	-3.18280600	-4.62936900	2.31992500
C	-0.60732500	3.54731600	2.29871500	H	-2.22761300	-5.20469600	0.09007300
C	-0.70355300	4.79278800	1.43137200	H	-0.28419600	-3.98685900	-0.78354100
C	-1.05283800	4.39410900	0.00710200	H	-0.15077300	-1.63182600	2.82592400
H	-1.60910200	3.08911300	2.37019300	H	-2.10281800	-2.84181400	3.68454800
H	-0.30727900	3.80768200	3.32824400	C	-1.67135600	-0.86291800	-2.37868800
H	-1.46503500	5.47775000	1.83284700	H	-1.16036600	0.11220700	-2.36729100
H	0.24367500	5.35623000	1.45158800	H	-1.04081200	-1.58142800	-1.82601100
H	-2.06883800	3.95761100	0.00816900	H	-1.70713300	-1.19391800	-3.42728300
H	-1.09460800	5.28042400	-0.64825900	C	-3.71557800	-2.15714600	-1.95954300
N	0.09370600	2.18833500	0.30428900	H	-3.65983200	-2.47290600	-3.01290500
C	-4.11101800	0.13936000	0.33150900	H	-3.18918800	-2.93043600	-1.37342800
C	-3.07131100	-0.76333300	-1.76930700	H	-4.77179300	-2.19038700	-1.66992300
C	-3.87617300	0.25763800	-2.59171000	C	-5.07088900	-0.97604400	0.80308300
C	-5.18334500	0.64742400	-1.91953500	H	-5.85623200	-0.57156300	1.46058300
C	-4.89923700	1.15419200	-0.51437300	H	-5.57589700	-1.49074000	-0.02179700

H -4.52915300 -1.74121500 1.38717100
C -3.64815300 0.85407100 1.60175100
H -3.08426400 0.17239100 2.26146800
H -3.00214100 1.71646500 1.36671900
H -4.49874600 1.24221100 2.18113400
C 1.80555400 3.00592100 2.01355800
H 1.93871600 4.06950000 1.78423600
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H 2.57080400 2.46725500 1.43071900
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H -0.86856300 3.67705300 -2.59899500
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H 1.77922800 1.03144200 -2.21500000
H 2.18961400 0.01547200 -3.59043100
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H 2.68704900 -2.63580400 -2.06888100
H 3.53318500 -1.90069500 -3.45299200
H 4.44082600 -2.39087000 -2.02023300
C 4.61062000 -2.18209300 0.66722600
H 5.16283600 -2.48267300 -0.22931700
H 5.29847400 -2.29833700 1.51887600
H 3.78275900 -2.89424100 0.80323300
C 3.60950300 -0.41238300 2.02929800
H 3.21196800 0.60923800 2.10491600
H 2.82580600 -1.11085500 2.36679200
H 4.44721500 -0.49022900 2.73762000
Li 1.65494300 0.99738800 -0.04448200
Li -1.36454800 0.88598200 -0.05348600

In situ deprotometallation using TMPCu and TMPLi

Control reaction 1: *In situ* study of TMPLi in C₆D₆

24 h



0 h

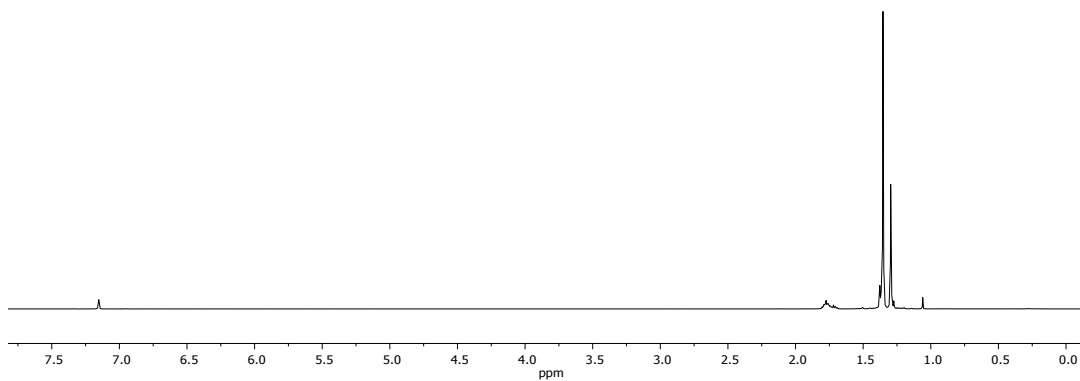
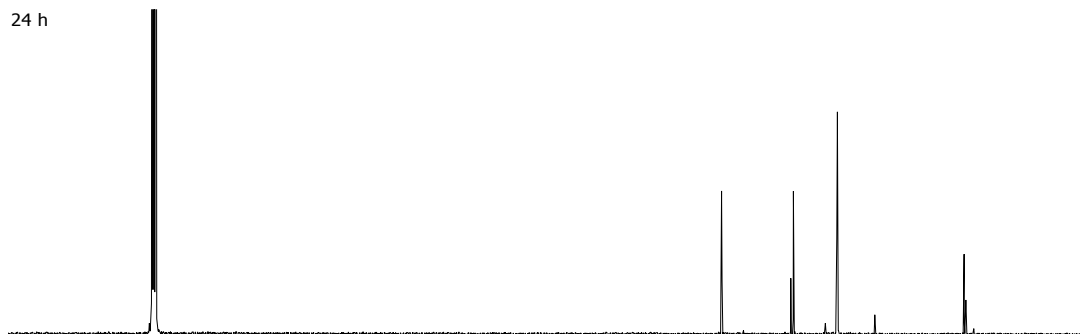


Figure S14a ¹H NMR spectrum of TMPLi before and after heating to 50°C for *ca.* 24 h.

24 h



0 h

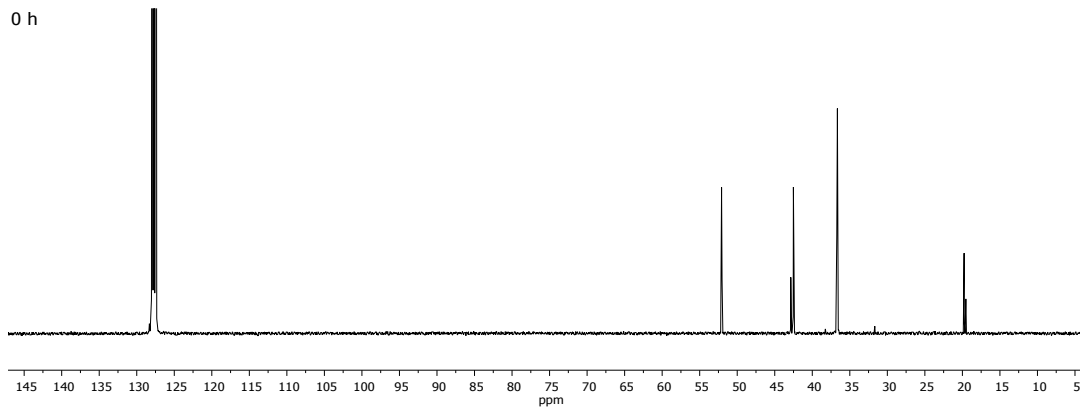
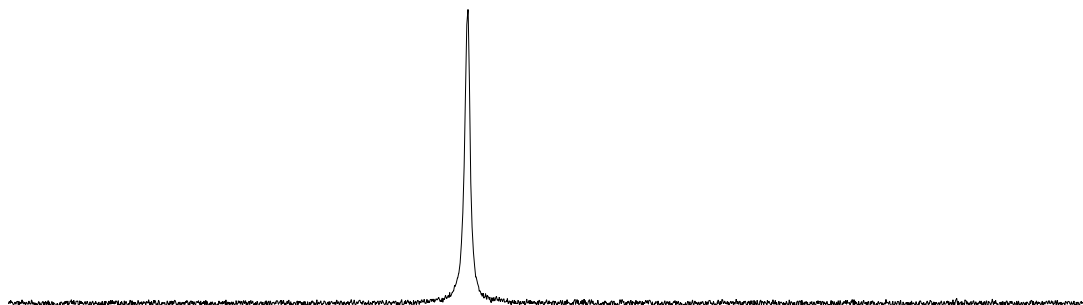


Figure S14b ¹³C NMR spectrum of TMPLi before and after heating to 50°C for *ca.* 24 h.

24 h



0 h

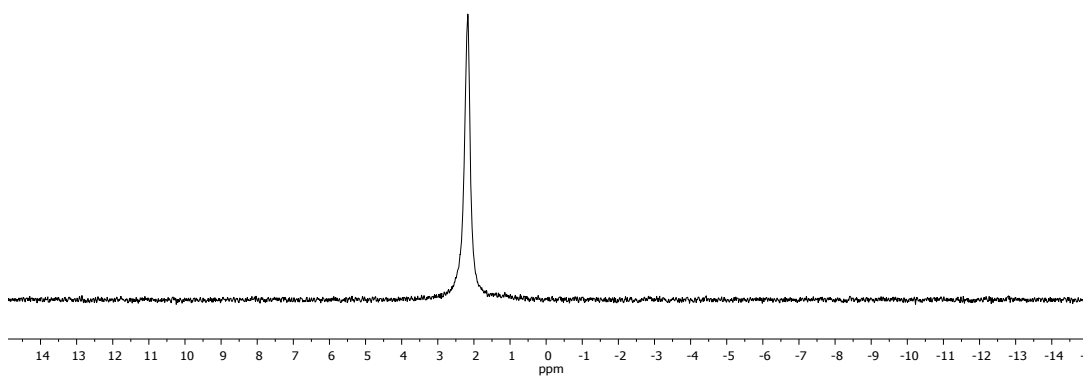


Figure S14c ^7Li NMR spectrum of TMPLi after heating to 50°C for *ca.* 24 h.

Control reaction 2: *In situ* study of TMPCu in C₆D₆

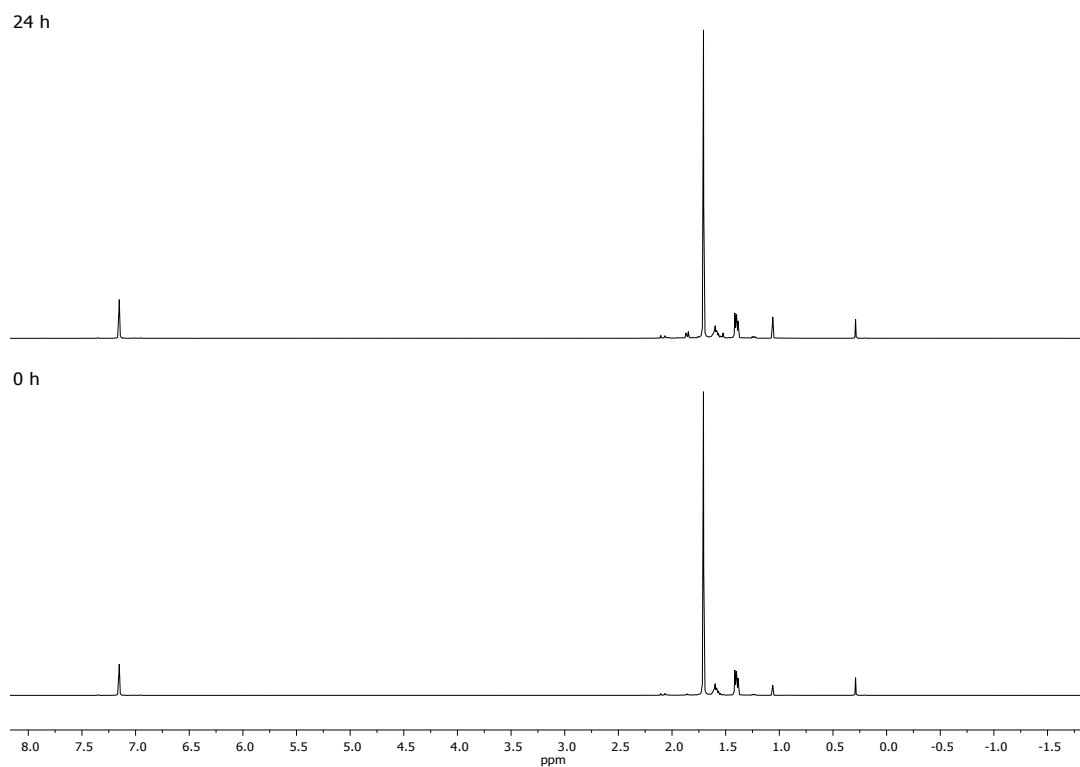


Figure S15a ¹H NMR spectrum of TMPCu before and after heating to 50°C for 24 h. In contrast to the reactivity shown by a mixture of TMPCu and TMPLi (main manuscript Figure 9 and below Figure S17) only a vanishingly small amount of **6** has formed as evidenced by the signals at δ 1.87, 1.85, 1.52 ppm.

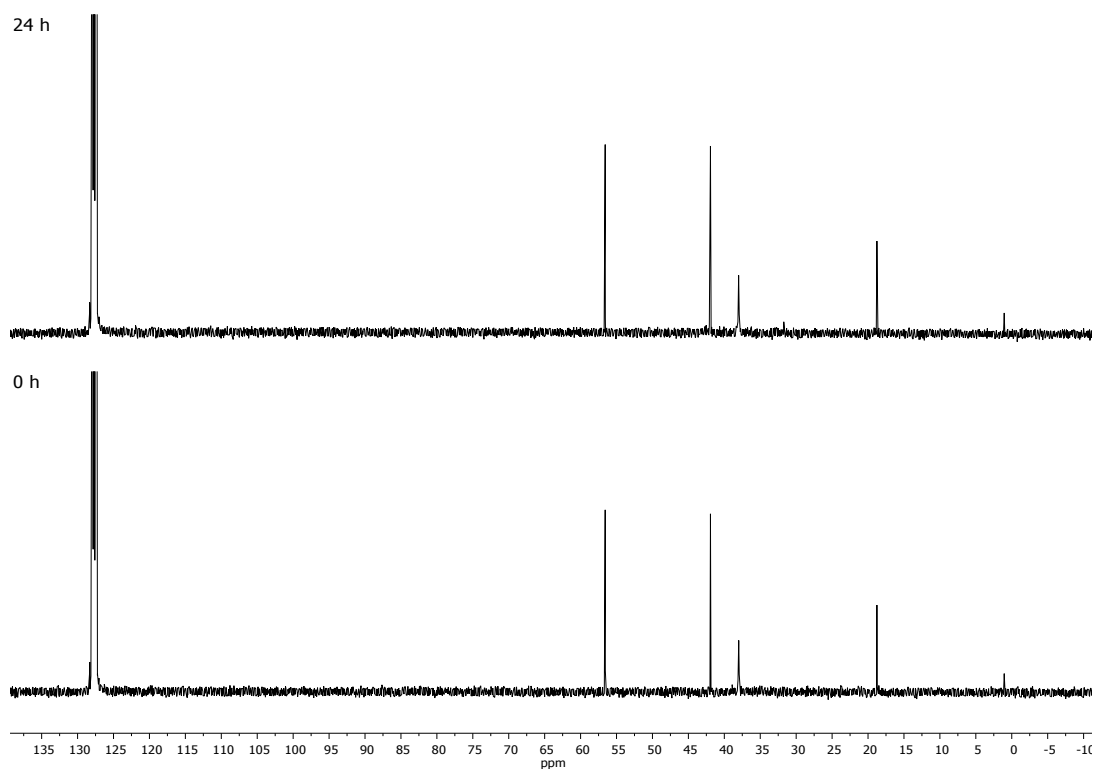


Figure S15b ¹³C NMR spectrum of TMPCu before and after heating to 50°C for 24 h.

Control reaction 3: *In situ* study of $\text{TMPCu}(\mu\text{-TMP})\text{Li}$ **2** in C_6D_6

24 h



0 h

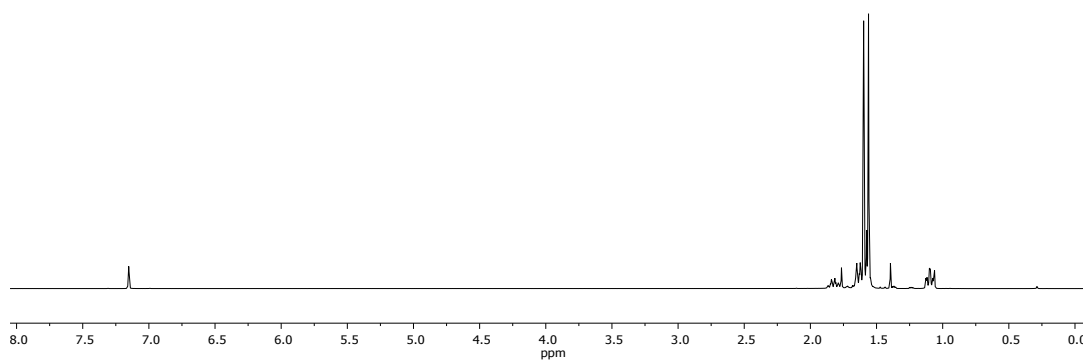
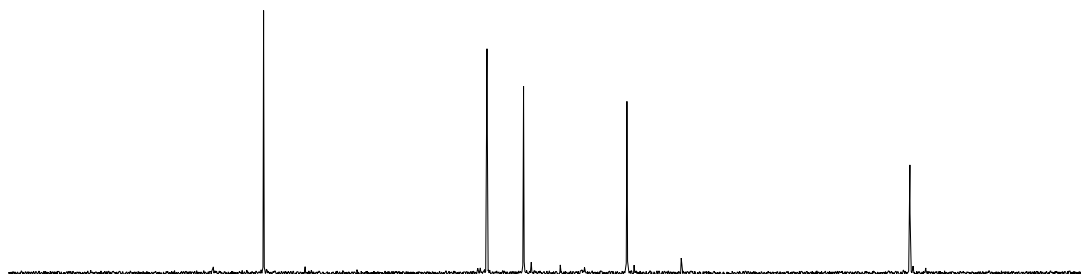


Figure S16a ^1H NMR spectrum of **2** before and after heating to 50°C for 24 h.

24 h



0 h

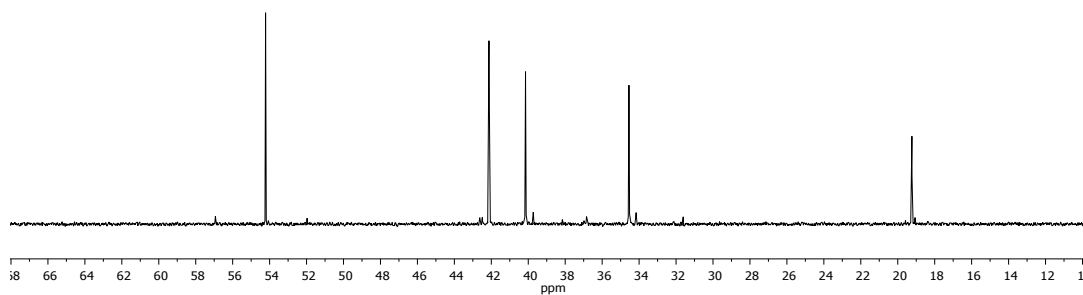


Figure S16b ^{13}C NMR spectrum of **2** before and after heating to 50°C for 24 h.

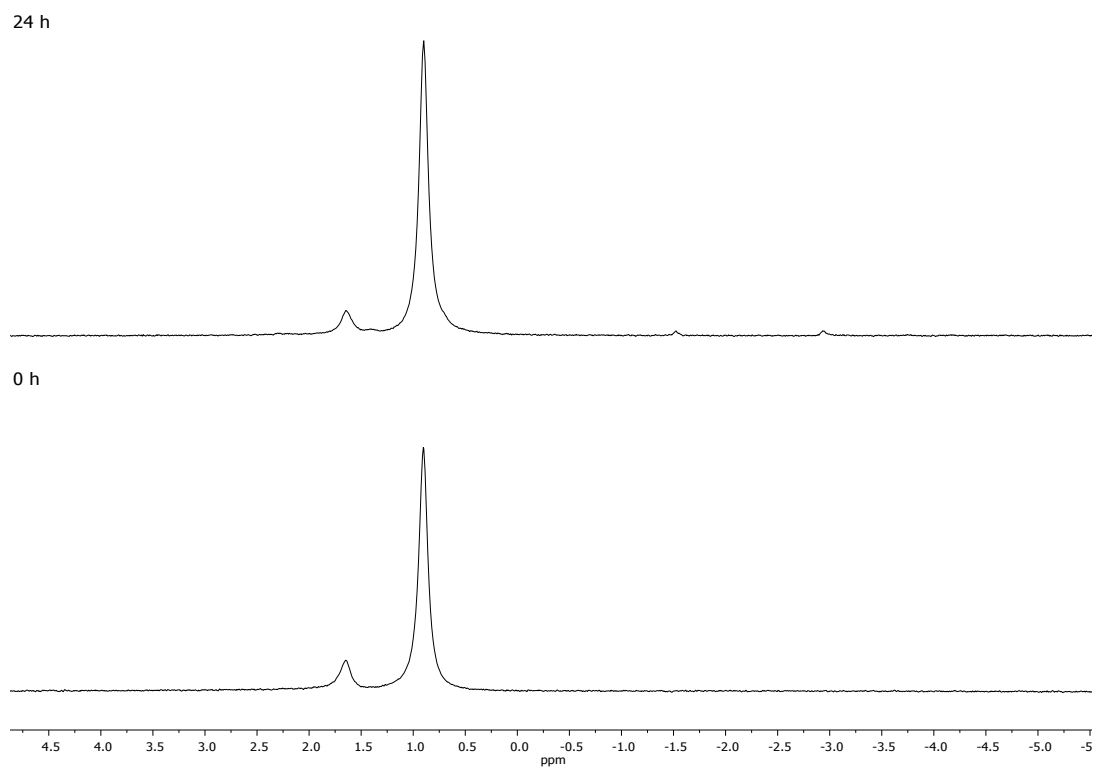


Figure S16c ^7Li NMR spectrum of **2** before and after heating to 50°C 24 h.

***In situ* reaction of TMPLi and TMPCu with C₆D₆**

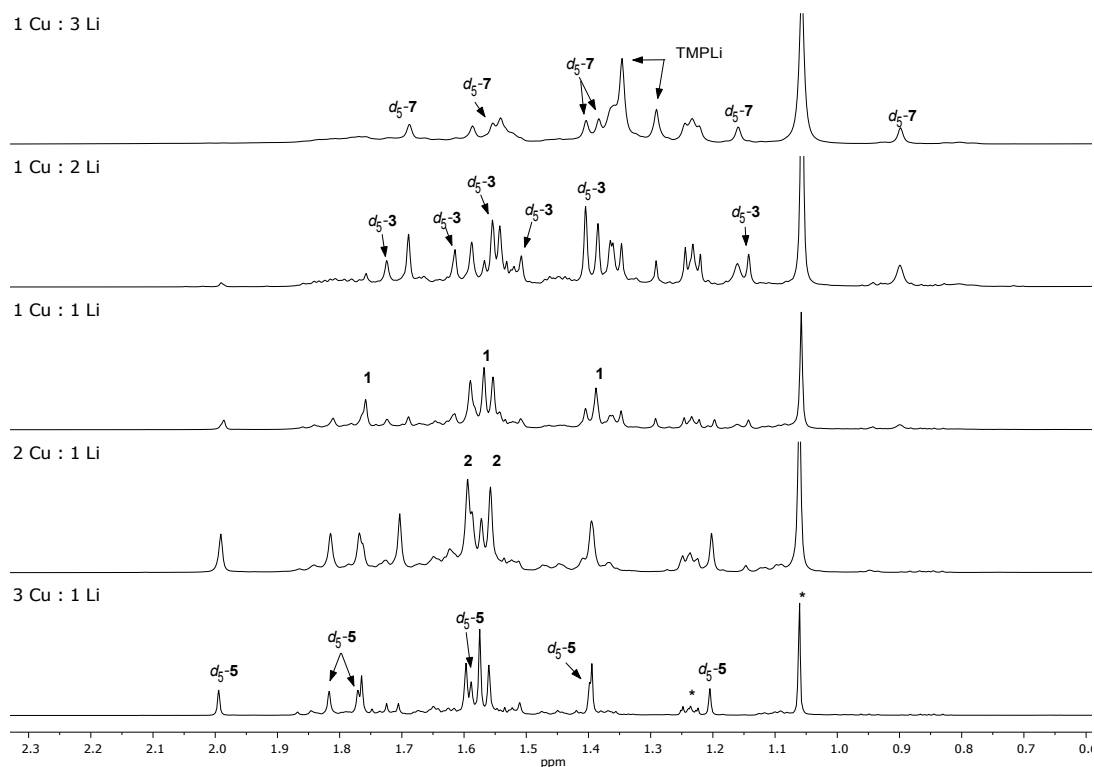


Figure S17a ¹H NMR spectra (500 MHz, 298 K, C₆D₆) of reaction mixtures containing TMPLi and TMPCu in the molar ratios specified and heated to 50°C for *ca.* 24 h. * = TMPLi.

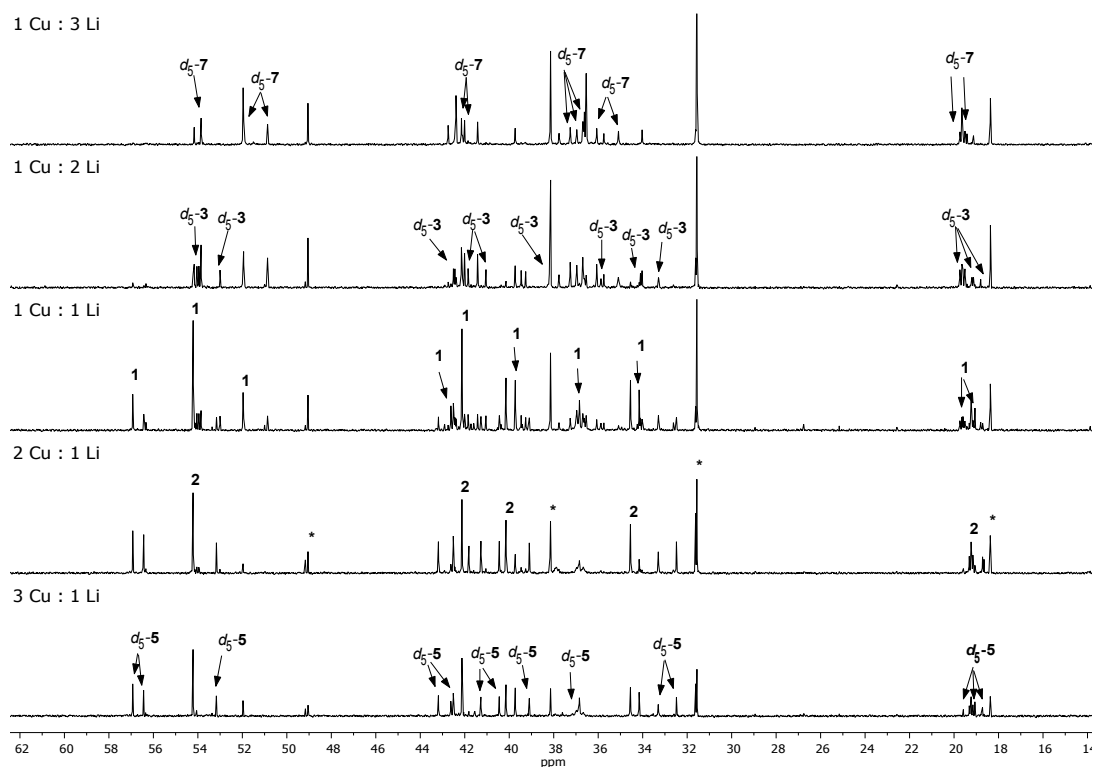


Figure S17b ¹³C NMR spectra (125 MHz, 298 K, C₆D₆) of reaction mixtures containing TMPLi and TMPCu in the molar ratios specified and heated to 50°C for *ca.* 24 h. * = TMPLi.

1:1 reaction of TMPLi and TMPCu with benzene

Experimental

TMPCu (203 mg, 1 mmol) and TMPLi (147 mg, 1 mmol) were combined in C₆H₆ (6 mL) and heated to 50°C for *ca.* 5 days, after which time the volatiles were removed *in vacuo* to leave a white residue.

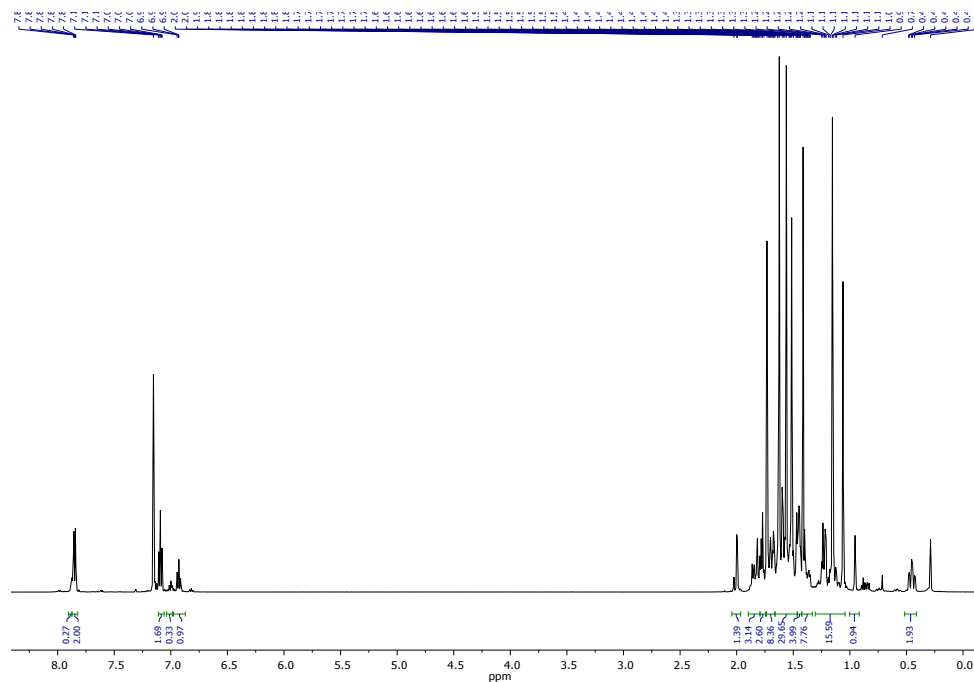


Figure S18a ¹H NMR spectrum (500 MHz, 298 K, C₆D₆) of an aliquot from the reaction mixture containing TMPCu and TMPLi (1:1) in C₆H₆, which was heated to 50°C for *ca.* 5 days.

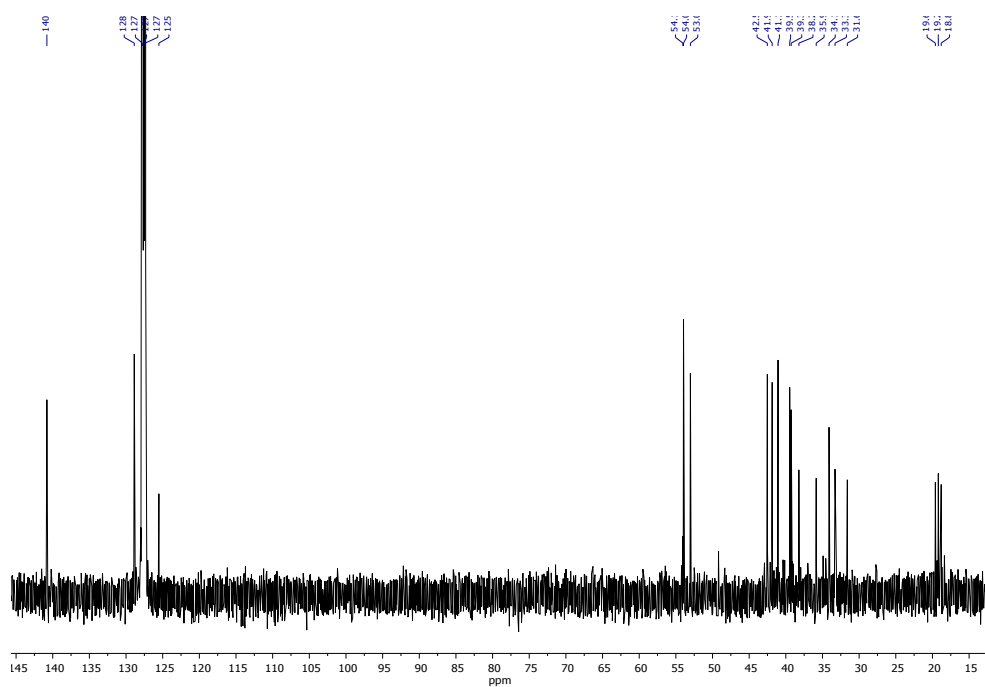


Figure S18b ^{13}C NMR spectrum (125 MHz, 298 K, C_6D_6) of an aliquot from the reaction mixture containing TMPCu and TMPLi (1:1) in C_6H_6 , which was heated to 50°C for *ca.* 5 days.

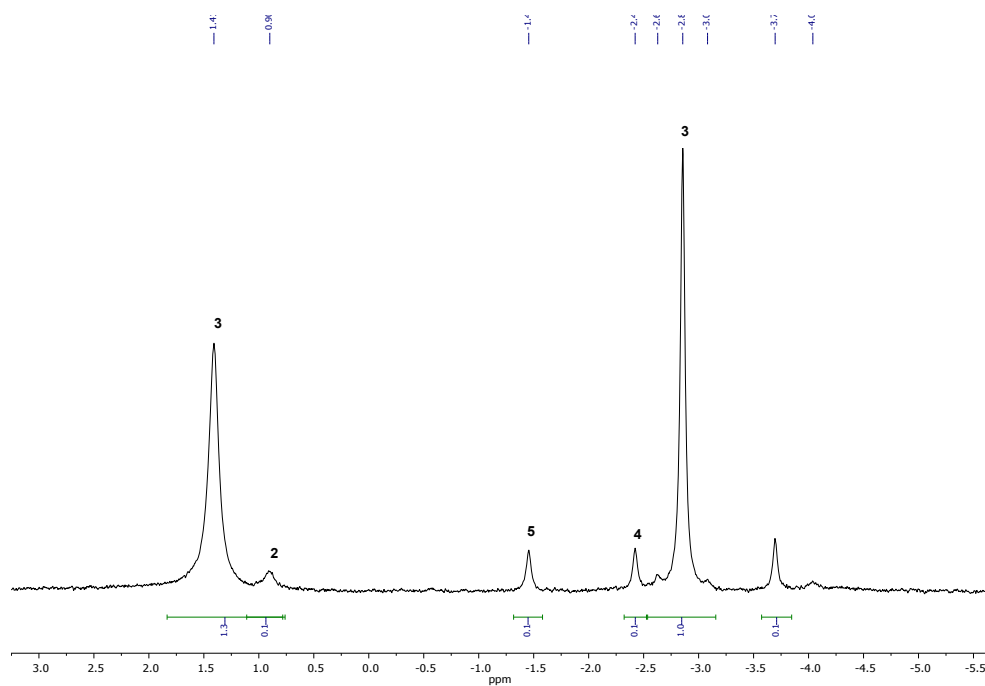


Figure S18c ^7Li NMR spectrum (194 MHz, C_6D_6) of an aliquot from the reaction mixture containing TMPCu and TMPLi (1:1) in C_6H_6 , which was heated to 50°C for *ca.* 5 days.