Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting information for:

Reversible hydrogen activation by a bulky haloborane based FLP system

Marc-André Courtemanche, Étienne Rochette,[a] Marc-André Légaré,[a] and Frédéric-Georges Fontaine[a]*

a) Département de Chimie, Université Laval, 1045 Avenue de la Médecine, Québec (Québec), Canada, G1V 0A6

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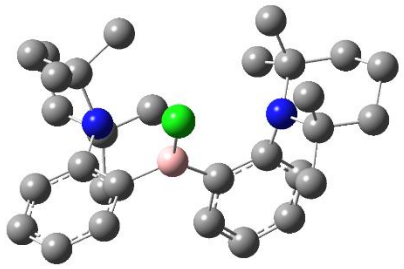
Cartesian coordinates and energies of optimized structures

1

Sum of electronic and thermal Free Energies= -1763.39

Sum of electronic and thermal Enthalpies= -1763.29

Wiberg bond indexes(B-N): 0.0054 and 0.0054



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C	**1.91139900**	**0.35435400**	**1.45044800**	**C**	**-4.57975700**	**-0.72306500**	**1.98003500**
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C	**3.15445800**	**0.60282800**	**0.85663800**	**C**	**-3.57685900**	**0.70767900**	**4.68517400**
C	**2.13102100**	**0.74674000**	**-1.31485500**	**C**	**-2.06352300**	**-1.21376700**	**4.87093500**
H	**0.00395100**	**0.50624100**	**-1.35972000**	**C**	**-5.66687500**	**-1.65126300**	**2.56527400**
C	**3.26999000**	**0.78806900**	**-0.51406900**	**C**	**-4.35018400**	**-1.09581900**	**0.50597700**
H	**4.03553300**	**0.65699700**	**1.48961400**	**C**	**-5.10481000**	**0.72879100**	**1.96608800**
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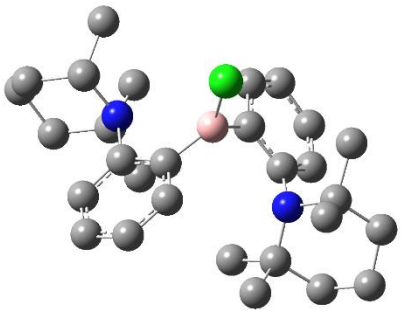
Cl	**-1.65682900**	**1.52731600**	**1.42226100**

1’

Sum of electronic and thermal Free Energies= -1763.39

Sum of electronic and thermal Enthalpies= -1763.3

Wiberg bond indexes (B-N): 0.00385 (left nitrogen) and 0.0040 (right nitrogen)



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C	**2.53372000**	**0.61402300**	**0.59369000**		**C**	**-4.42476100**	**-2.49215100**	**-1.32547500**
C	**1.20194500**	**1.42568100**	**-1.24008500**		**C**	**-3.80779600**	**-0.05069600**	**-1.66729800**
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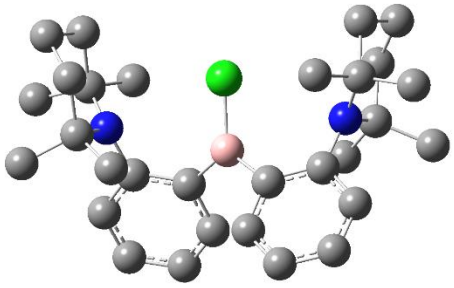
Cl	**-2.21841000**	**1.70913800**	**2.04298300**

1’’

Sum of electronic and thermal Free Energies= -1763.4

Sum of electronic and thermal Enthalpies= -1763.3

Wiberg bond indexes (B-N): 0.0396 (left nitrogen) and 0.0387 (right nitrogen)



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C	**16.46663100**	**2.99160900**	**0.18035300**	**H**	**12.68952000**	**0.33492500**	**2.88386400**
C	**17.06876100**	**3.50794000**	**-0.98212800**	**H**	**14.37764600**	**0.69701700**	**3.25571300**
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H	**16.59552300**	**0.71647900**	**-1.22510600**
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C	**19.57618800**	**-0.81727600**	**-1.56409600**
H	**20.12128800**	**-1.47642700**	**-2.23293300**
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C	**21.25266500**	**2.77596600**	**2.94975900**
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C	**20.47477700**	**-0.07359500**	**2.68258300**
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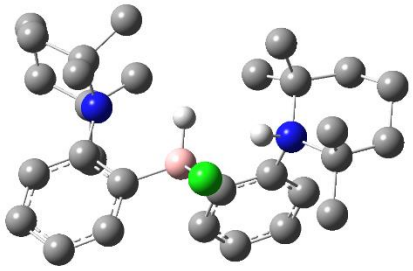
2

Sum of electronic and thermal Free Energies= -1764.57

Sum of electronic and thermal Enthalpies= -1764.48



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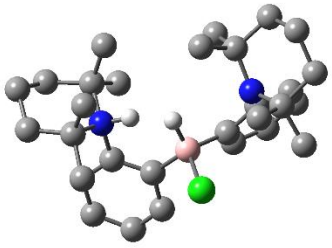
C	**2.23835600**	**0.55961300**	**0.87991000**	**C**	**-3.21329600**	**0.26928100**	**4.65269600**
C	**1.01494000**	**-0.70348700**	**-0.75078800**	**C**	**-3.32148000**	**-2.17975400**	**4.79746300**
H	**-0.35172900**	**-2.15765900**	**0.02584600**	**C**	**-5.28875300**	**-0.18909900**	**1.51463300**
C	**1.94192800**	**0.28855600**	**-0.44924500**	**C**	**-3.33848400**	**-0.76487000**	**0.07386000**
H	**2.96591900**	**1.32501700**	**1.11947700**	**C**	**-3.15304200**	**1.17119000**	**1.54324400**
H	**0.78338900**	**-0.93395900**	**-1.78592900**	**C**	**-5.83613400**	**0.08580200**	**2.91062500**
H	**2.43751100**	**0.84506500**	**-1.23774600**	**H**	**-5.66320100**	**-0.74930000**	**4.90503600**
C	**-1.42812500**	**-2.82739900**	**2.24801600**	**H**	**-5.65652900**	**-1.93903200**	**3.60842200**
C	**-2.77836800**	**-2.44024600**	**2.16531600**	**H**	**-3.46697500**	**0.21015300**	**5.71619600**
C	**-1.10693400**	**-4.12928500**	**1.83004000**	**H**	**-2.12671200**	**0.31649300**	**4.56124200**
C	**-3.74267000**	**-3.36161300**	**1.73053000**	**H**	**-3.63500000**	**1.20313900**	**4.27971100**
C	**-2.05908200**	**-5.02726100**	**1.36662000**	**H**	**-2.23416800**	**-2.25019100**	**4.88081000**
H	**-0.06974800**	**-4.44852900**	**1.89016100**	**H**	**-3.73739800**	**-2.03931300**	**5.80009600**
C	**-3.39553900**	**-4.64249900**	**1.32577900**	**H**	**-3.69446700**	**-3.12893300**	**4.40961000**
H	**-4.78519000**	**-3.05899100**	**1.70846500**	**H**	**-5.63871800**	**0.57040700**	**0.80525900**
H	**-1.76405200**	**-6.02485400**	**1.05423400**	**H**	**-5.68988200**	**-1.14828200**	**1.16307000**
H	**-4.16123000**	**-5.33395300**	**0.98633500**	**H**	**-3.67693400**	**-0.04130000**	**-0.67440000**

H	**-2.25244800**	**-0.85389900**	**-0.00695900**
H	**-3.77927500**	**-1.73232900**	**-0.16789800**
H	**-2.07149700**	**1.11174400**	**1.40377900**
H	**-3.56648800**	**1.79353300**	**0.74226400**
H	**-3.34806600**	**1.67917400**	**2.48599200**
H	**-6.93091900**	**0.04949800**	**2.89805500**
H	**-5.56818300**	**1.10055500**	**3.23030800**
N	**1.91956000**	**0.11113200**	**3.30844900**
C	**1.28170200**	**1.43405600**	**3.84526800**
C	**3.40946700**	**-0.17634500**	**3.71524300**
C	**2.27542300**	**2.59264400**	**3.69897200**
C	**0.85665100**	**1.20205700**	**5.30199600**
C	**0.02149100**	**1.76129700**	**3.04023300**
C	**4.26520800**	**1.08833100**	**3.57433200**
C	**3.95866700**	**-1.29540100**	**2.82396200**
C	**3.43558400**	**-0.67921200**	**5.16821900**
C	**3.66822600**	**2.31762100**	**4.25001700**
H	**1.82611600**	**3.45801200**	**4.19681600**
H	**2.35218800**	**2.85692300**	**2.63801400**
H	**0.19075400**	**2.01494700**	**5.60013100**
H	**0.29657900**	**0.26683400**	**5.39968200**
H	**1.68692700**	**1.18748200**	**6.00572100**
H	**-0.69740900**	**0.94310600**	**3.07114100**
H	**-0.44250500**	**2.64193900**	**3.49244100**
H	**0.24159100**	**1.99335000**	**1.99777200**
H	**5.24363900**	**0.85142800**	**4.00459500**
H	**4.44407900**	**1.30002000**	**2.51525400**
H	**4.95204500**	**-1.55687400**	**3.19807000**
H	**3.32477900**	**-2.18338200**	**2.87473400**
H	**4.05968900**	**-0.99107200**	**1.78256300**
H	**2.69409300**	**-1.46442200**	**5.33009000**
H	**4.42114900**	**-1.11268100**	**5.35282000**
H	**3.29036700**	**0.10909800**	**5.90466200**
H	**4.31092900**	**3.18415900**	**4.06994400**
H	**3.63351300**	**2.18343200**	**5.33618600**
Cl	**0.94845800**	**-2.90777900**	**3.95561600**
H	**-0.68100700**	**-1.01772200**	**3.56996000**
H	**1.41008300**	**-0.64584600**	**3.78974300**

2’



Sum of electronic and thermal Enthalpies= -1764.476802

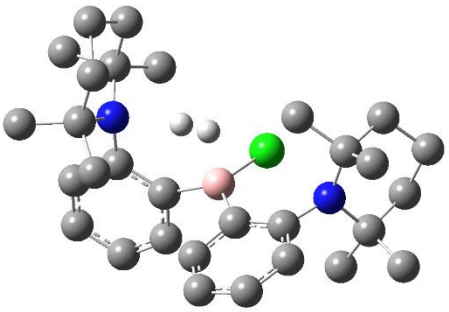
Sum of electronic and thermal Free Energies= -1764.571514

B	**-0.66251400**	**-0.19616200**	**1.33513300**	**C**	**-1.88005200**	**-2.45344600**	**4.20343300**
C	**0.87702800**	**-0.05408800**	**0.80713400**	**C**	**-5.75494600**	**-1.28589700**	**2.77980600**
C	**1.96057900**	**0.22735300**	**1.63976800**	**C**	**-4.69869400**	**-0.61201700**	**0.62398500**
C	**1.18382400**	**-0.15087400**	**-0.56209200**	**C**	**-4.59945300**	**0.94494600**	**2.53206600**
C	**3.27344900**	**0.35249100**	**1.18381200**	**C**	**-5.62134100**	**-1.48076200**	**4.28660400**
C	**2.47621200**	**-0.03137200**	**-1.04836800**	**N**	**1.62044800**	**0.44953400**	**3.06486300**
C	**3.53230800**	**0.20915600**	**-0.16978300**	**C**	**1.76655700**	**1.92640200**	**3.51893600**
C	**-1.35305000**	**-1.63949100**	**1.05803500**	**C**	**2.12517800**	**-0.64836800**	**4.03145700**
C	**-2.58192300**	**-2.02032500**	**1.64596500**	**C**	**3.18868500**	**2.16160000**	**4.04217600**
C	**-0.72377800**	**-2.60390700**	**0.25281700**	**C**	**0.70416600**	**2.22477900**	**4.58758900**
C	**-3.13331800**	**-3.27796700**	**1.37279900**	**C**	**1.47104800**	**2.84401200**	**2.32617000**
C	**-1.27151900**	**-3.85594800**	**-0.00869800**	**C**	**3.54049200**	**-0.29986000**	**4.50614100**
C	**-2.49779500**	**-4.19479900**	**0.54612800**	**C**	**2.11150900**	**-1.98440500**	**3.27879800**
N	**-3.24754600**	**-1.14990800**	**2.57735200**	**C**	**1.16121300**	**-0.76547500**	**5.22669000**
C	**-3.07183700**	**-1.49976800**	**4.01536800**	**C**	**3.66914800**	**1.12208500**	**5.05465000**
C	**-4.54904200**	**-0.55051400**	**2.15180500**	**Cl**	**-1.58490000**	**1.26937700**	**0.49839200**
C	**-4.31705300**	**-2.20622800**	**4.59790100**	**H**	**-0.75581800**	**0.04163000**	**2.54318600**
C	**-2.75091200**	**-0.23272100**	**4.84154000**	**H**	**0.58581200**	**0.29896200**	**3.01272900**

H_2 activation TS (B-Cl)

Sum of electronic and thermal Enthalpies= -1764.447429

Sum of electronic and thermal Free Energies= -1764.543327



B	17.05140200	1.17652900	0.90614400	H	11.68687100	2.81908000	3.52789200
C	16.36532100	2.41532100	0.17497600	H	12.04682300	1.36957100	4.44865200
C	17.04233000	2.86025300	-0.97583100	C	13.78895100	2.56187400	4.00585100
H	17.90181900	2.29913800	-1.32138400	H	14.46503000	1.71778800	4.18468400
C	16.66364200	3.98272600	-1.69995200	H	13.74331400	3.14564900	4.93236000
H	17.22493000	4.27739100	-2.58086300	C	14.40995300	3.43949300	2.90197800
C	15.56638600	4.71628300	-1.27691900	C	15.87821500	3.66611400	3.28812200
H	15.25246100	5.60723700	-1.81240500	H	16.38901200	2.70847800	3.40604400
C	14.85018600	4.28637200	-0.16618800	H	15.92635700	4.19323200	4.24578600
H	13.97363200	4.84174000	0.14241100	H	16.41089800	4.26966800	2.54726600
C	15.20365800	3.13985900	0.55770100	C	13.72838100	4.82850800	2.89677000
N	14.35320600	2.69394800	1.61943100	H	14.19280700	5.49453400	2.16551800
C	13.39242900	1.06012700	0.02751600	H	13.84371100	5.29640100	3.88015400
H	13.71377600	1.58305500	-0.87719300	H	12.66011400	4.77654600	2.68416600
H	12.48060700	0.50494500	-0.21402500	C	18.22885200	0.39284800	0.16422300
H	14.16489600	0.34442300	0.31244200	C	17.75263800	-0.37619300	-0.91084200
C	11.98563000	2.98845600	0.66333000	H	16.68915300	-0.35378700	-1.13836000
H	11.65368200	3.70615200	1.41394200	C	18.58590200	-1.15570800	-1.69997800
H	11.11143500	2.40043200	0.36456200	H	18.17513600	-1.73265600	-2.52227200
H	12.31808800	3.54131100	-0.21810900	C	19.94725900	-1.18326200	-1.42530100
C	13.09058200	2.03466800	1.17813100	H	20.62068300	-1.78370900	-2.02872900
C	12.54040300	1.20611200	2.35336100	C	20.44558000	-0.43607000	-0.36680000
H	11.57190200	0.78487400	2.06127300	H	21.50688800	-0.46731700	-0.15545400
H	13.22345300	0.36702200	2.52602700	C	19.61416600	0.35346600	0.43950300
C	12.41831900	2.00934900	3.64113800	N	20.16844200	1.10760400	1.53894100

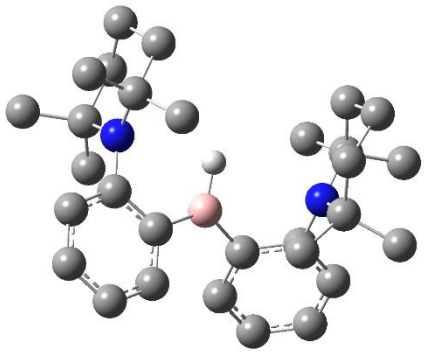
C	**20.19378400**	**3.13437800**	**0.12759100**
H	**20.12775100**	**2.60615300**	**-0.82685300**
H	**20.71502300**	**4.07977800**	**-0.04930500**
H	**19.18206300**	**3.36836600**	**0.46327400**
C	**22.36567500**	**2.05638200**	**0.57024100**
H	**23.04039000**	**1.53488500**	**1.24828500**
H	**22.83101200**	**3.01565900**	**0.32239300**
H	**22.29510600**	**1.48342100**	**-0.35645600**
C	**20.96856900**	**2.32153500**	**1.17224700**
C	**21.10358700**	**3.20223900**	**2.42872900**
H	**21.74695700**	**4.05501500**	**2.18578900**
H	**20.11410100**	**3.61012100**	**2.67170400**
C	**21.63192500**	**2.44914000**	**3.64103300**
H	**22.65742100**	**2.10273500**	**3.46599500**
H	**21.67526500**	**3.11730600**	**4.50731300**
C	**20.70909100**	**1.27476400**	**3.93166100**
H	**19.71385300**	**1.66411400**	**4.18186600**
H	**21.05736600**	**0.70813000**	**4.80187100**
C	**20.56144900**	**0.30516500**	**2.74421500**
C	**19.43009800**	**-0.66984700**	**3.08866700**
H	**18.48413600**	**-0.14985700**	**3.24104500**
H	**19.68205600**	**-1.19384100**	**4.01551500**
H	**19.28076400**	**-1.41979900**	**2.30803600**
C	**21.84490700**	**-0.54116400**	**2.59798000**
H	**21.74248800**	**-1.28276300**	**1.80295000**
H	**22.01194000**	**-1.08950900**	**3.53038800**
H	**22.74042100**	**0.04932600**	**2.40590200**
Cl	**16.15984600**	**0.13554300**	**2.09758200**
H	**18.50809400**	**1.90229700**	**2.01037900**
H	**17.81532700**	**2.24575300**	**2.09934600**

3

Sum of electronic and thermal Free Energies= -1303.76

Sum of electronic and thermal Enthalpies= -1303.67

Wiberg bond indexes (N-B): 0.008 (left nitrogen) 0.0837 (right nitrogen)



C	**13.50835000**	**3.17236600**	**8.32335000**	**C**	**15.85869300**	**-0.38502300**	**10.58192700**
H	**14.50993700**	**3.60378200**	**8.42010100**	**H**	**15.90644600**	**-1.10742400**	**9.76286300**
H	**12.78398700**	**3.99135700**	**8.36553700**	**H**	**16.07607900**	**-0.91629100**	**11.51384000**
H	**13.42787100**	**2.70055300**	**7.34092800**	**H**	**16.63484100**	**0.36836300**	**10.42533500**
C	**11.78751200**	**1.64397100**	**9.24736300**	**C**	**13.43653100**	**-0.84892500**	**10.88274600**
H	**11.73387700**	**1.07113000**	**8.31744100**	**H**	**12.42516000**	**-0.46777800**	**11.03285800**
H	**11.07385600**	**2.47097700**	**9.16833300**	**H**	**13.69766800**	**-1.44741200**	**11.76227600**
H	**11.45578000**	**0.99968400**	**10.06317300**	**H**	**13.42460700**	**-1.52260300**	**10.02255700**
C	**13.21696400**	**2.18765300**	**9.46739400**	**N**	**14.25328800**	**1.13153200**	**9.49770000**
C	**13.28412800**	**2.99360400**	**10.77763800**	**C**	**14.68966000**	**0.61563200**	**8.24128000**
H	**14.20255900**	**3.59428400**	**10.75828000**	**C**	**13.98066600**	**-0.39259700**	**7.58140300**
H	**12.44053600**	**3.69252500**	**10.80316300**	**H**	**13.07067300**	**-0.77998600**	**8.02554100**
C	**13.30872700**	**2.11982700**	**12.02361100**	**C**	**14.42413400**	**-0.90238800**	**6.36358700**
H	**13.38555900**	**2.74535300**	**12.91919400**	**H**	**13.85986300**	**-1.69068700**	**5.87380400**
H	**12.37340300**	**1.55537200**	**12.12142000**	**C**	**15.58104400**	**-0.40303300**	**5.77636000**
C	**14.50213700**	**1.17840100**	**11.93893400**	**H**	**15.93289300**	**-0.80239600**	**4.83042600**
H	**14.56357200**	**0.54133100**	**12.82843100**	**C**	**16.27911700**	**0.61501500**	**6.41421700**
H	**15.42017300**	**1.77957300**	**11.90540500**	**H**	**17.18359500**	**1.00729700**	**5.95721100**
C	**14.47592200**	**0.27838500**	**10.68927400**	**C**	**15.86247400**	**1.14325500**	**7.64663100**

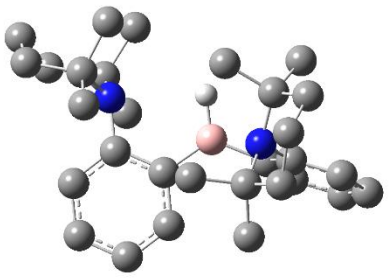
B	**16.69643300**	**2.24801500**	**8.36195100**
H	**16.50116000**	**2.43869300**	**9.52058900**
C	**19.53335000**	**0.60077800**	**8.34184200**
H	**18.46962000**	**0.38853400**	**8.48449700**
H	**20.07032000**	**-0.35191100**	**8.37778800**
H	**19.66923800**	**1.02785800**	**7.34490100**
C	**21.57135800**	**1.74464000**	**9.16051400**
H	**21.70948100**	**2.30008700**	**8.22932700**
H	**22.07352800**	**0.77852300**	**9.04495800**
H	**22.08014400**	**2.28361000**	**9.96099800**
C	**20.06922200**	**1.52311600**	**9.44757200**
C	**19.89194200**	**0.76812200**	**10.77868700**
H	**18.88003500**	**0.34543000**	**10.79892300**
H	**20.59130100**	**-0.07543300**	**10.79402800**
C	**20.06893600**	**1.64337200**	**12.01108400**
H	**19.87578800**	**1.05743000**	**12.91580300**
H	**21.10230600**	**2.00183000**	**12.09092400**
C	**19.10067800**	**2.81477900**	**11.92730900**
H	**19.18297200**	**3.45649200**	**12.81161400**
H	**18.07522300**	**2.42368500**	**11.90032900**
C	**19.31315300**	**3.67462200**	**10.66858600**
C	**18.14700900**	**4.67275800**	**10.59043300**
H	**18.26116800**	**5.36980400**	**9.75627400**
H	**18.11588200**	**5.25827500**	**11.51462800**
H	**17.19342700**	**4.15386900**	**10.47748600**
C	**20.60583200**	**4.50932800**	**10.82203500**
H	**21.50434700**	**3.89908200**	**10.91710200**
H	**20.53365500**	**5.12903700**	**11.72211400**
H	**20.74008600**	**5.18604200**	**9.97519300**
N	**19.26439100**	**2.77205000**	**9.48754700**
C	**18.99116200**	**3.39283200**	**8.22484300**
C	**19.91555000**	**4.21532100**	**7.57490700**
H	**20.88554700**	**4.39290800**	**8.02445600**
C	**19.60970900**	**4.80176100**	**6.34941400**
H	**20.33941400**	**5.44174900**	**5.86245500**
C	**18.38147600**	**4.55776300**	**5.74566300**
H	**18.14232300**	**5.01161900**	**4.78906400**
C	**17.46930600**	**3.71443300**	**6.37165700**
H	**16.51461400**	**3.50980800**	**5.89333400**
C	**17.74443000**	**3.13451300**	**7.61794100**

3’

Sum of electronic and thermal Free Energies= -1303.75

Sum of electronic and thermal Enthalpies= -1303.66

Wiberg bond indexes (N-B): 0.0303 (left nitrogen)0.0087 (right nitrogen)



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C	**1.85807900**	**0.35718100**	**1.48434200**	**C**	**-4.31473200**	**-0.62430500**	**1.71549900**
C	**0.83468000**	**0.12464100**	**-0.68456000**	**C**	**-4.76762500**	**-1.70154000**	**4.45707100**
C	**3.02644000**	**0.82482200**	**0.88160900**	**C**	**-3.36729700**	**0.39959400**	**4.60564700**
C	**2.00019700**	**0.58748600**	**-1.28840500**	**C**	**-2.28243500**	**-1.79541600**	**4.78700500**
H	**-0.01568600**	**-0.15417300**	**-1.30247500**	**C**	**-5.63981000**	**-1.30223400**	**2.12810500**
C	**3.09445300**	**0.94328900**	**-0.50339600**	**C**	**-4.02947100**	**-0.97976400**	**0.24694300**
H	**3.88470200**	**1.08354500**	**1.49450700**	**C**	**-4.45410000**	**0.91156200**	**1.74764600**
H	**2.05883300**	**0.67066900**	**-2.36928900**	**C**	**-5.93631800**	**-1.17992500**	**3.62194900**
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C	**-0.44607800**	**-2.85475600**	**0.82626500**	**H**	**-2.57814900**	**0.95515300**	**4.09475300**
C	**-2.83215500**	**-3.45746200**	**2.07769100**	**H**	**-4.30456500**	**0.94163000**	**4.47810000**
C	**-0.89945200**	**-4.16561800**	**0.82408400**	**H**	**-1.31882100**	**-1.33092500**	**4.56198000**
H	**0.48132900**	**-2.61231000**	**0.31439600**	**H**	**-2.44403200**	**-1.73400900**	**5.86689100**
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3''

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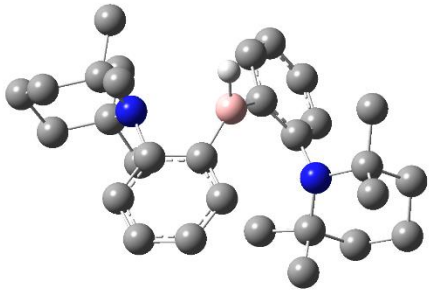
Sum of electronic and thermal Enthalpies= -1303.65

Wiberg bond indexes (N-B): 0.0991 (left nitrogen) 0.0119 (right nitrogen)



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C	**1.31029000**	**0.50491500**	**1.62773800**	**C**	**-1.50452100**	**-1.78418800**	**-1.63551400**
C	**-0.12265500**	**1.62362700**	**0.03626200**	**C**	**-4.43010600**	**-2.23956600**	**-1.56042800**
C	**2.40327700**	**1.11334200**	**0.99342400**	**C**	**-3.98663700**	**0.24636500**	**-1.30463400**
C	**0.96496300**	**2.21563600**	**-0.58832600**	**C**	**-4.56880600**	**-1.11294200**	**0.65544300**
H	**-1.12578000**	**1.85427700**	**-0.31344300**	**C**	**-2.18202100**	**-2.88458300**	**-2.47990700**
C	**2.24165100**	**1.93658700**	**-0.11344200**	**C**	**-0.12408200**	**-2.27077100**	**-1.17688500**
H	**3.39968500**	**0.96396300**	**1.38790100**	**C**	**-1.23179800**	**-0.55950700**	**-2.53095200**
H	**0.81965900**	**2.89507900**	**-1.42204300**	**C**	**-3.63314300**	**-2.55392400**	**-2.82349900**
H	**3.11245600**	**2.39069500**	**-0.57644700**	**H**	**-5.44950700**	**-1.93015500**	**-1.81982300**
C	**-1.56176700**	**-1.49292100**	**1.84201700**	**H**	**-4.52987000**	**-3.15539600**	**-0.96475200**
C	**-2.08281600**	**-2.20257700**	**0.75681900**	**H**	**-5.03535200**	**0.54422700**	**-1.21217700**
C	**-1.41458500**	**-2.14511900**	**3.06726900**	**H**	**-3.37305100**	**0.97863100**	**-0.77407700**
C	**-2.38681000**	**-3.56091000**	**0.88496000**	**H**	**-3.73776100**	**0.28889900**	**-2.36389600**
C	**-1.73652600**	**-3.49107500**	**3.20333000**	**H**	**-4.18444600**	**-0.33847000**	**1.32284600**
H	**-1.03966000**	**-1.59513600**	**3.92270200**	**H**	**-5.61567000**	**-0.88369200**	**0.43576300**
C	**-2.20645900**	**-4.20434700**	**2.10437300**	**H**	**-4.54133900**	**-2.06702200**	**1.18324600**
H	**-2.78079400**	**-4.11462100**	**0.04079100**	**H**	**-1.59961200**	**-3.03024800**	**-3.39729100**
H	**-1.61196400**	**-3.98469200**	**4.16231300**	**H**	**-2.14095700**	**-3.83649000**	**-1.93754500**
H	**-2.44576700**	**-5.25892500**	**2.19983200**	**H**	**0.48260800**	**-2.49764700**	**-2.05833600**

H	**0.38429300**	**-1.48936300**	**-0.60619800**
H	**-0.17408600**	**-3.17314800**	**-0.56527900**
H	**-0.89261800**	**0.28401700**	**-1.93084700**
H	**-0.43821000**	**-0.81164700**	**-3.24063200**
H	**-2.09155200**	**-0.24528200**	**-3.12024800**
H	**-4.09357900**	**-3.39623400**	**-3.35055400**
H	**-3.67241100**	**-1.70627900**	**-3.51769800**
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C	**2.38451900**	**-1.39145500**	**2.85162000**
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C	**0.80426300**	**2.03230100**	**3.80245000**
C	**3.84918600**	**-1.01037000**	**3.16821300**
C	**2.30229600**	**-2.06746000**	**1.47689200**
C	**1.94611500**	**-2.47810300**	**3.85667000**
C	**3.97173000**	**-0.12849200**	**4.41048800**
H	**3.11249500**	**1.67798600**	**5.23739700**
H	**3.40051600**	**1.74327200**	**3.50689800**
H	**0.91300200**	**0.87535800**	**6.10325800**
H	**-0.08758000**	**-0.19015700**	**5.10911000**
H	**1.47779700**	**-0.73940700**	**5.71536600**
H	**-0.25854100**	**1.84295700**	**3.62497000**
H	**0.89065200**	**2.65558700**	**4.69717100**
H	**1.19327400**	**2.60305600**	**2.95774300**
H	**4.42477000**	**-1.93353200**	**3.30377800**
H	**4.29900800**	**-0.50010100**	**2.30975300**
H	**2.93700700**	**-2.95827700**	**1.47602400**
H	**1.27300000**	**-2.37879300**	**1.27996000**
H	**2.63231800**	**-1.42268700**	**0.66111500**
H	**0.87731100**	**-2.66617800**	**3.77520000**
H	**2.47191100**	**-3.40786400**	**3.61886400**
H	**2.18591100**	**-2.24407100**	**4.89286500**
H	**5.00945300**	**0.19852300**	**4.53494200**
H	**3.72988400**	**-0.70841400**	**5.30907300**
H	**-2.26267800**	**0.76648700**	**1.62622600**

H_2 activation TS (B-H)

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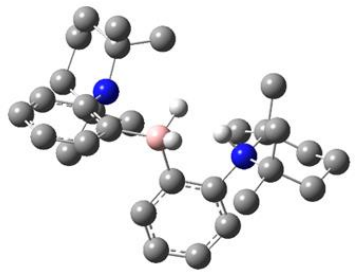
Sum of electronic and thermal Enthalpies= -1304.83



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C	**0.66570700**	**0.23380400**	**0.71585000**	**C**	**-3.40071400**	**0.56285200**	**4.51410000**
C	**1.81215100**	**0.32728500**	**1.52902900**	**C**	**-2.07194800**	**-1.51685100**	**4.69185200**
C	**0.85521500**	**0.43425500**	**-0.66279200**	**C**	**-5.64785200**	**-1.48423600**	**2.26993400**
C	**3.05352500**	**0.65152100**	**0.96299000**	**C**	**-4.23232600**	**-1.13779000**	**0.23399700**
C	**2.09237800**	**0.71860400**	**-1.22844400**	**C**	**-4.73161100**	**0.81622700**	**1.66011300**
H	**-0.01539900**	**0.36991700**	**-1.31175700**	**C**	**-5.84864400**	**-1.29550800**	**3.76965700**
C	**3.20632100**	**0.83817100**	**-0.40390200**	**H**	**-4.70119500**	**-1.49783900**	**5.59989600**
H	**3.91459100**	**0.75223900**	**1.61808900**	**H**	**-4.40135500**	**-2.75467000**	**4.41664400**
H	**2.18573600**	**0.86133000**	**-2.30145900**	**H**	**-3.17142600**	**0.61507500**	**5.58061700**
H	**4.18127200**	**1.07803800**	**-0.81830900**	**H**	**-2.65711100**	**1.16896200**	**3.98929300**
C	**-1.20039500**	**-1.65705400**	**1.35051900**	**H**	**-4.38099300**	**1.01551600**	**4.37487300**
C	**-2.36199700**	**-2.07795600**	**2.00522800**	**H**	**-1.17747300**	**-1.02397300**	**4.30747900**
C	**-0.44527600**	**-2.68547800**	**0.76795100**	**H**	**-2.11080700**	**-1.36390900**	**5.77348100**
C	**-2.75692300**	**-3.40576500**	**2.12692300**	**H**	**-1.98360000**	**-2.58625400**	**4.50059200**
C	**-0.80578000**	**-4.02420200**	**0.86904200**	**H**	**-6.54453200**	**-1.18111400**	**1.71973600**
H	**0.44802600**	**-2.41009400**	**0.21406900**	**H**	**-5.50012800**	**-2.54880600**	**2.05505700**
C	**-1.96029400**	**-4.39144300**	**1.55786800**	**H**	**-5.12050200**	**-0.86216800**	**-0.34141800**
H	**-3.66742100**	**-3.68027600**	**2.64754400**	**H**	**-3.36660300**	**-0.62992800**	**-0.19558700**
H	**-0.18632500**	**-4.78798600**	**0.40854600**	**H**	**-4.08940400**	**-2.21448000**	**0.14243800**
H	**-2.24437100**	**-5.43479600**	**1.64631000**	**H**	**-3.82251900**	**1.35698200**	**1.38042600**
N	**-3.19375300**	**-0.96584200**	**2.52912800**	**H**	**-5.48698400**	**1.02190600**	**0.89816600**
C	**-3.33495300**	**-0.91076800**	**4.07609400**	**H**	**-5.10653600**	**1.21524100**	**2.60042700**
C	**-4.47003000**	**-0.69643800**	**1.68381900**	**H**	**-6.68112800**	**-1.91854900**	**4.10928000**

H	**-6.13203800**	**-0.26099800**	**3.99146700**
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C	**1.64602900**	**1.35729100**	**3.78283200**
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C	**3.00184700**	**1.67392800**	**4.45055600**
C	**0.55240400**	**1.24567000**	**4.86573800**
C	**1.25098600**	**2.57048800**	**2.92400300**
C	**3.74773700**	**-0.68643500**	**4.22177400**
C	**2.79614100**	**-2.07705200**	**2.39713200**
C	**1.51174500**	**-1.85699100**	**4.45641100**
C	**3.59011500**	**0.47845800**	**5.19062300**
H	**2.87647900**	**2.52652600**	**5.12909700**
H	**3.70796400**	**1.99133400**	**3.67157900**
H	**0.42059400**	**2.21303300**	**5.36257400**
H	**-0.39003200**	**0.96874700**	**4.39121600**
H	**0.77747500**	**0.51529800**	**5.64303000**
H	**1.16868400**	**3.44532100**	**3.57710400**
H	**1.99186100**	**2.79144200**	**2.15415200**
H	**4.14303500**	**-1.57022000**	**4.73662100**
H	**4.49166000**	**-0.40932400**	**3.46352800**
H	**3.22814600**	**-2.96543200**	**2.86864100**
H	**1.90610800**	**-2.38533200**	**1.84651700**
H	**3.52258500**	**-1.68715100**	**1.68371000**
H	**0.62047100**	**-2.17030400**	**3.90675300**
H	**2.02219200**	**-2.75492900**	**4.82136200**
H	**1.19594800**	**-1.28715400**	**5.32989500**
H	**4.56081400**	**0.74097000**	**5.62518800**
H	**2.94593100**	**0.19257300**	**6.03156300**
H	**-1.05068600**	**0.45901000**	**2.33716100**
H	**-2.55105000**	**-0.17088000**	**2.32731200**
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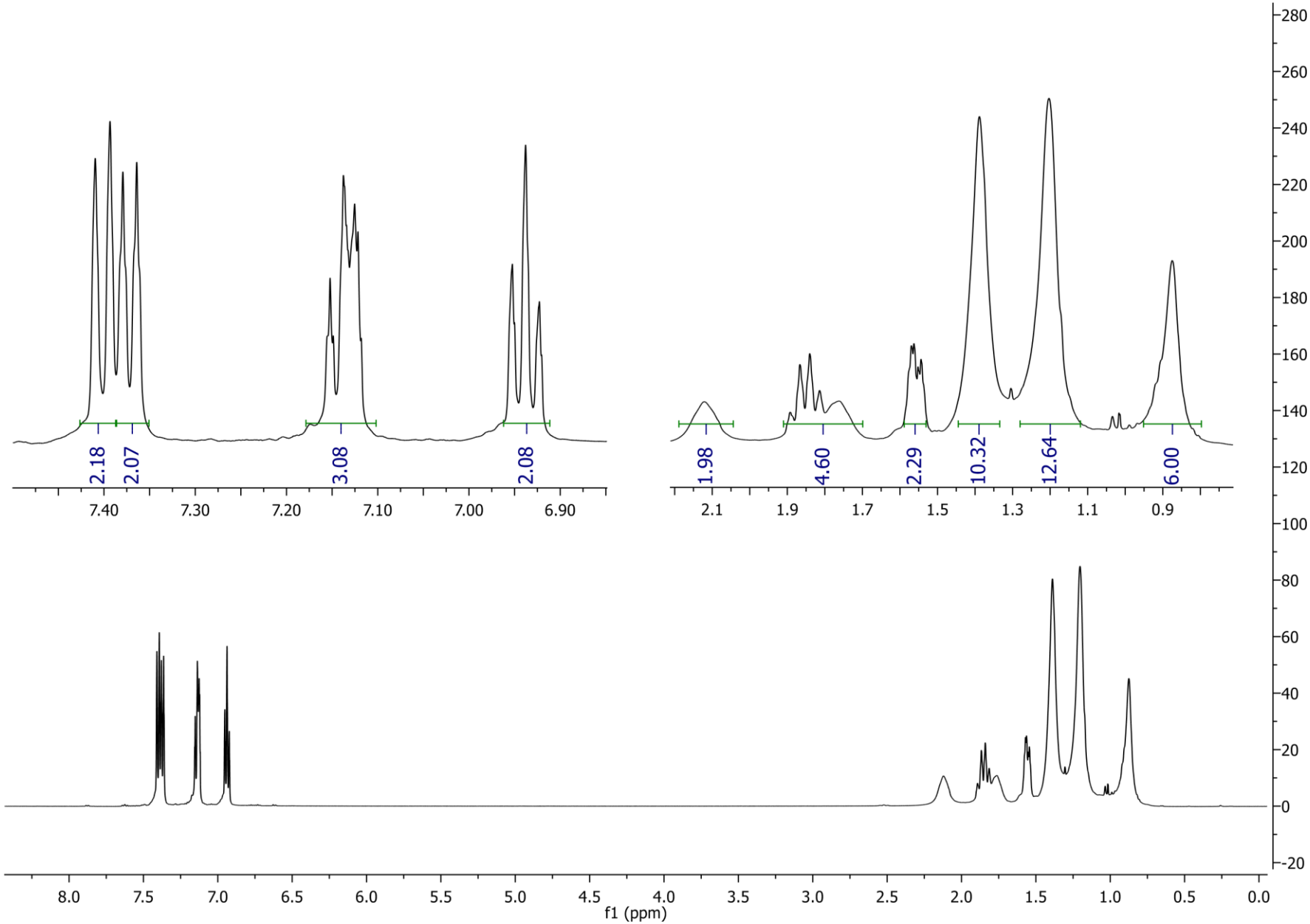

Figure S1. [1] H-NMR spectrum (500 MHz, benzene-d_6) of **1**.

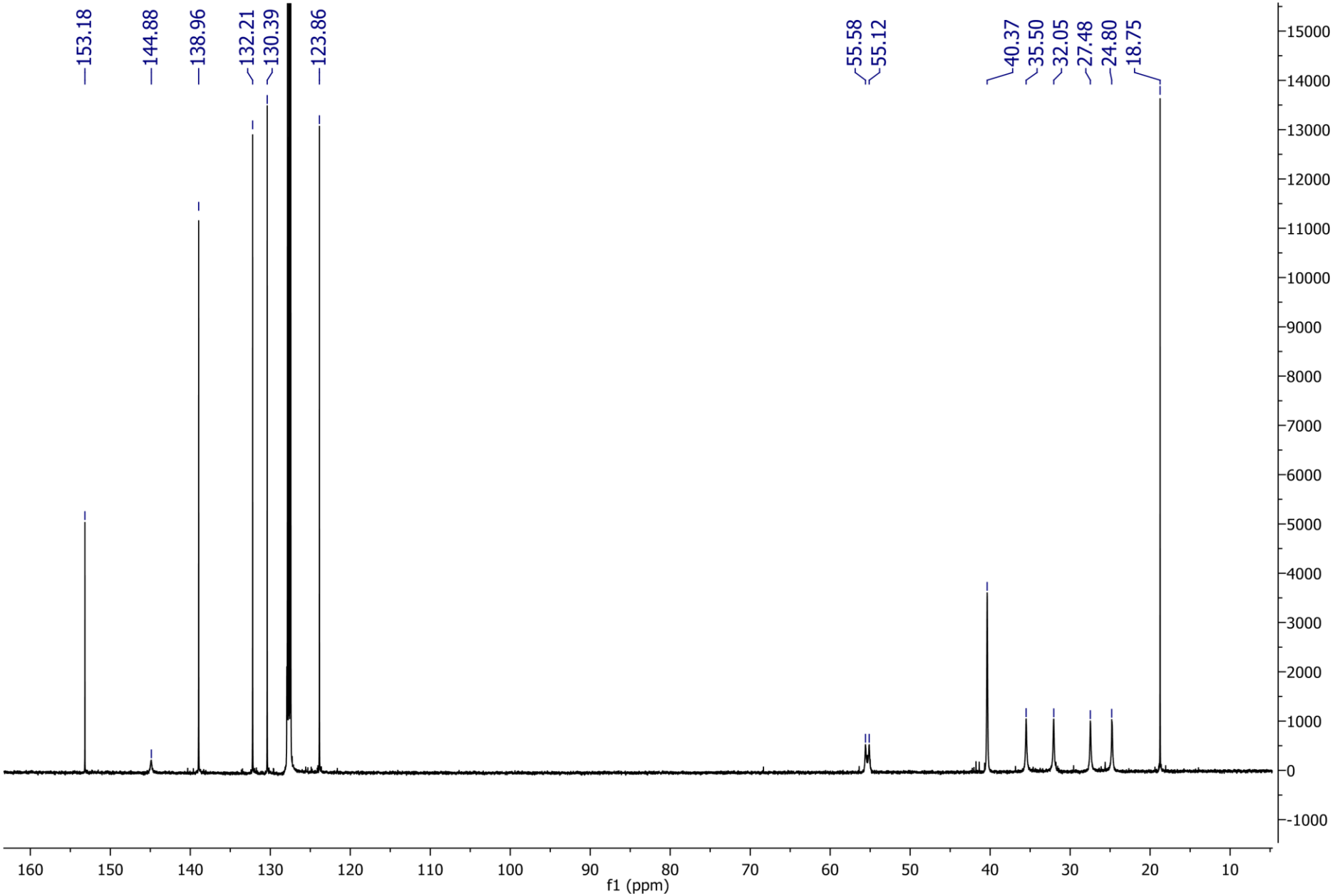

Figure S2. ^{13}C {^{1}H} NMR spectrum (126 MHz, benzene-*d*6) of **1**.

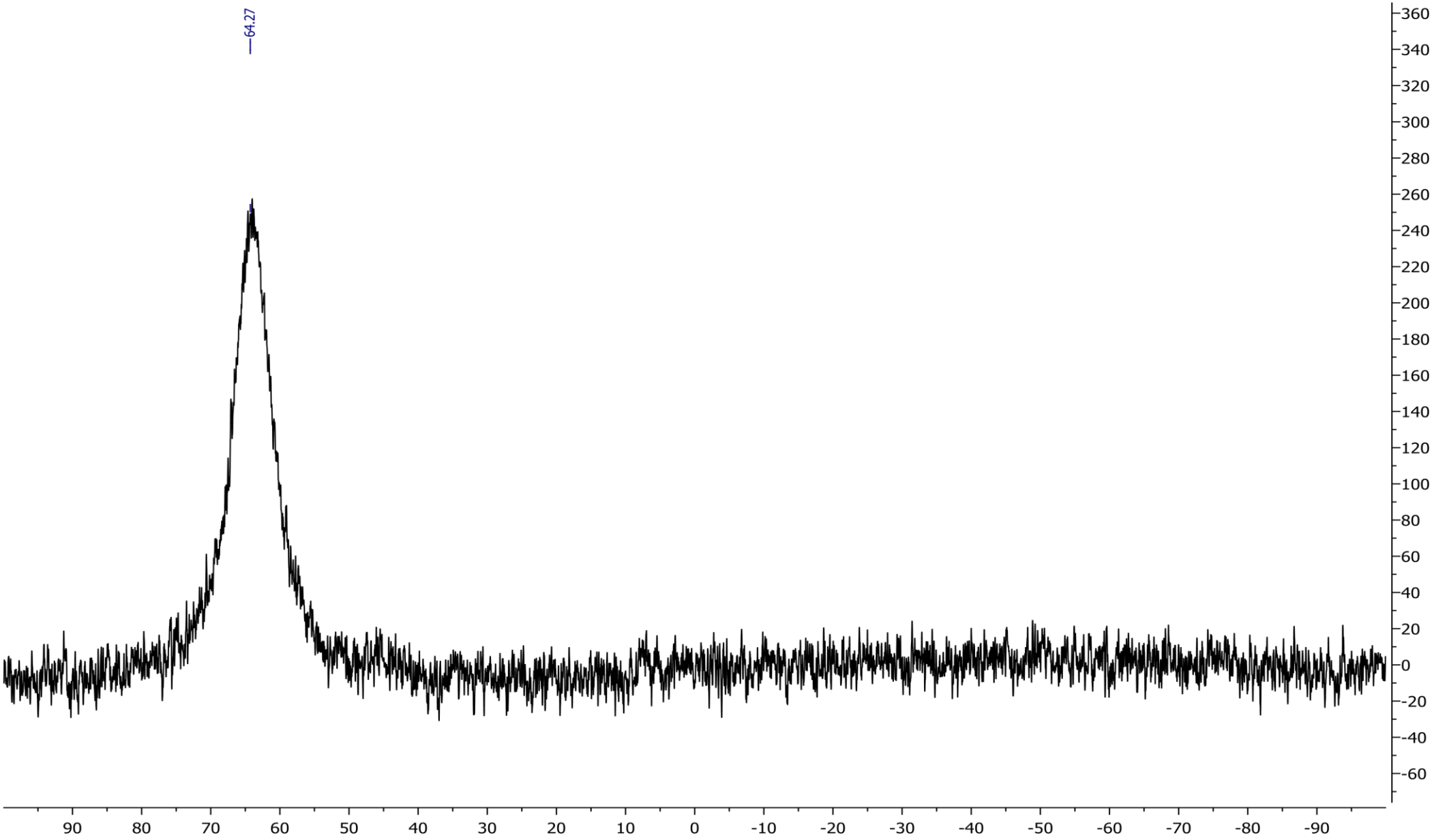

Figure S3. ^{11}B {^{1}H} NMR spectrum (160 MHz, benzene-*d*6) of **1**.

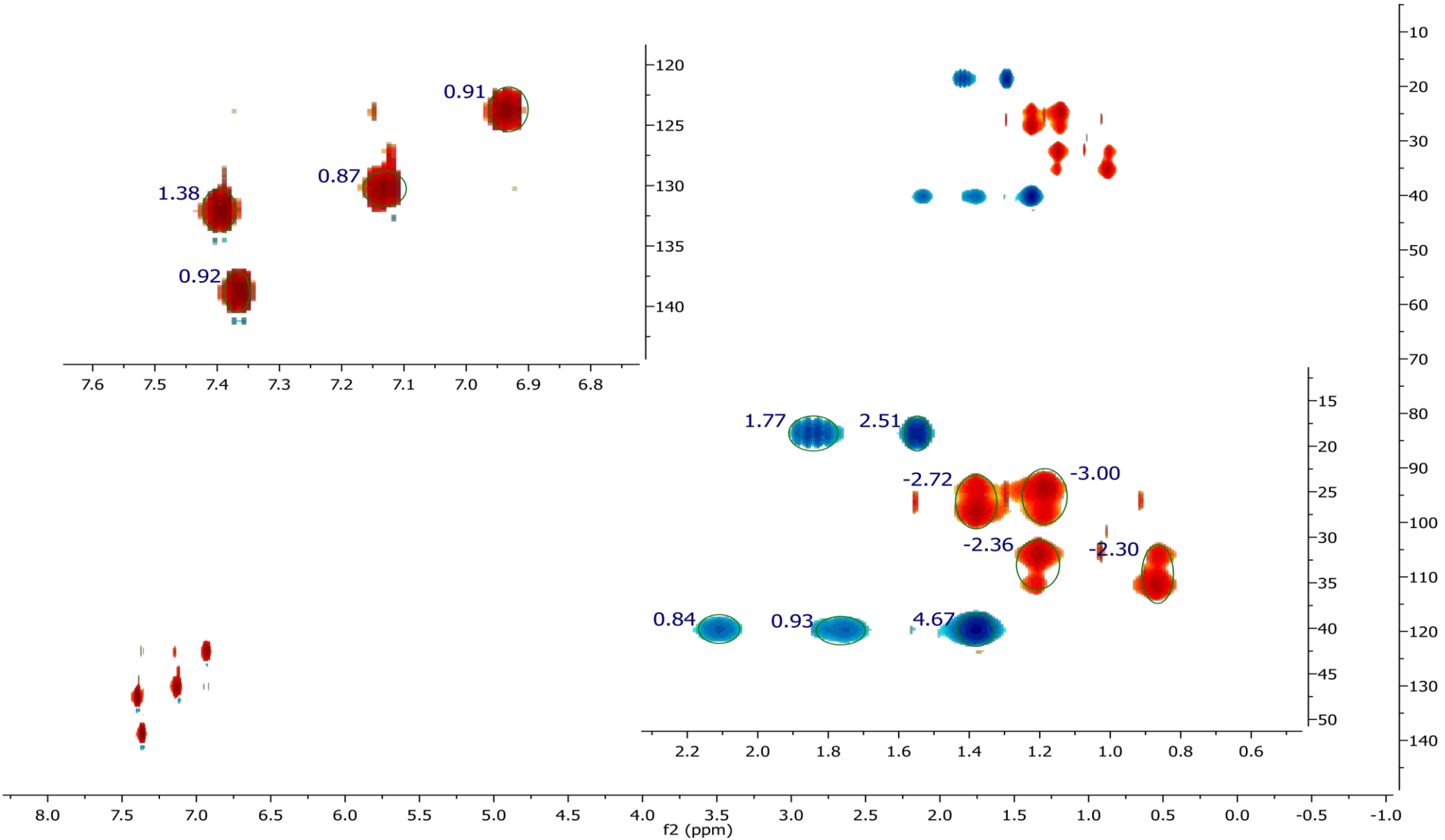

Figure S4. ^{13}C-^{1}H HSQC NMR spectrum (126 MHz–500 MHz, benzene-d_6) of **1**.

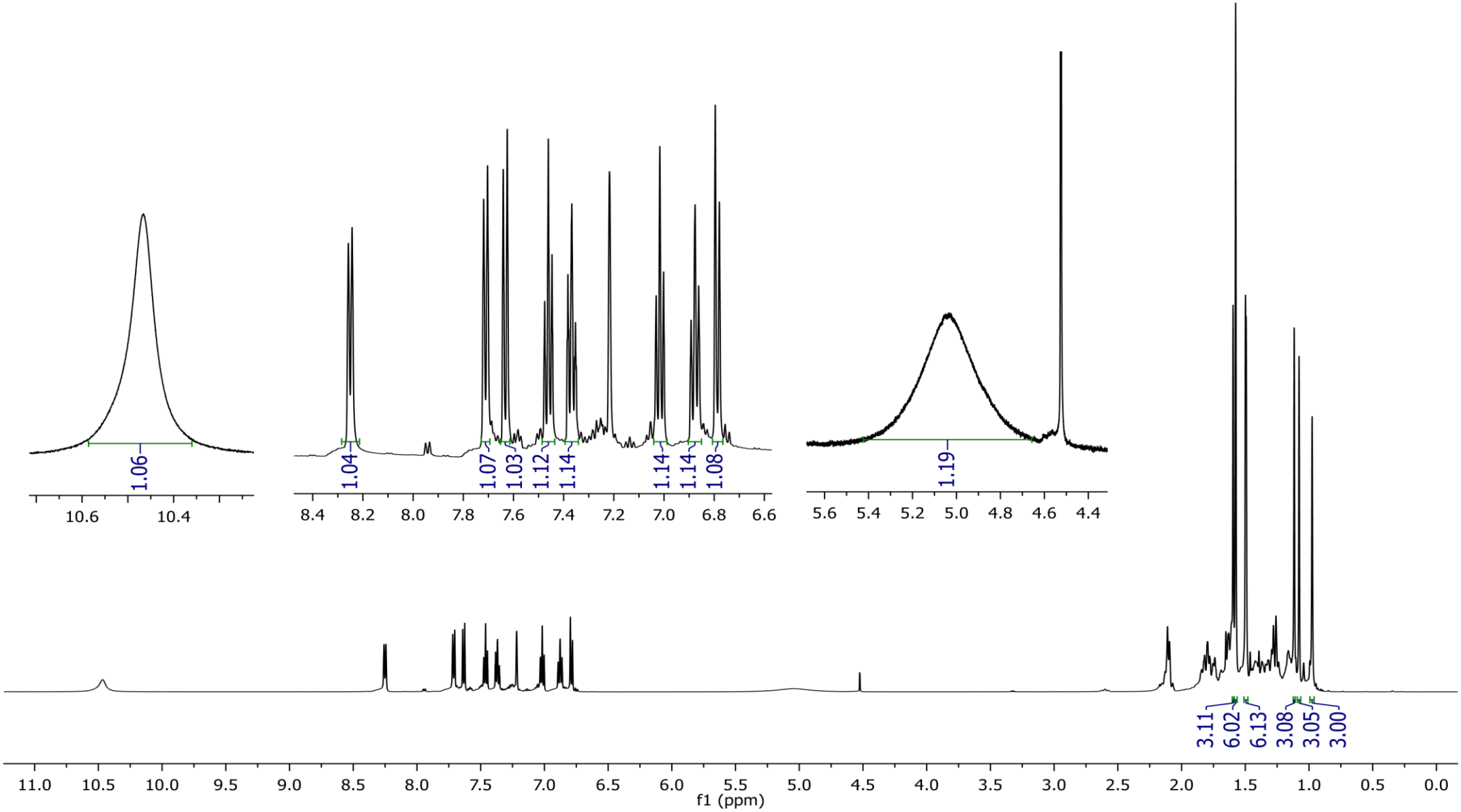

Figure S5. [1] H-NMR spectrum (500 MHz, benzene-d_6) of **2**.

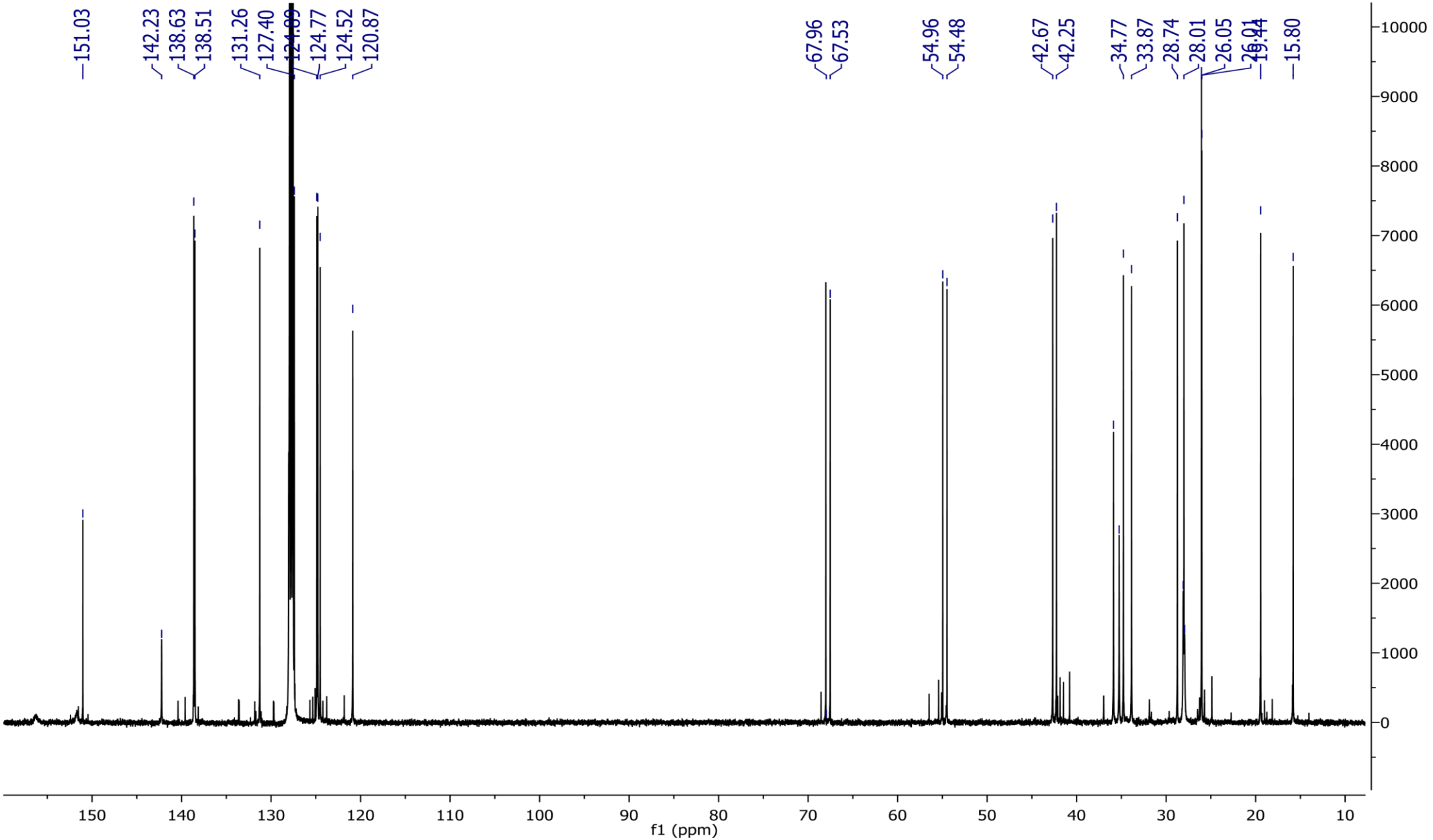

Figure S6. ^{13}C {^{1}H} NMR spectrum (126 MHz, benzene-*d*6) of **2**.

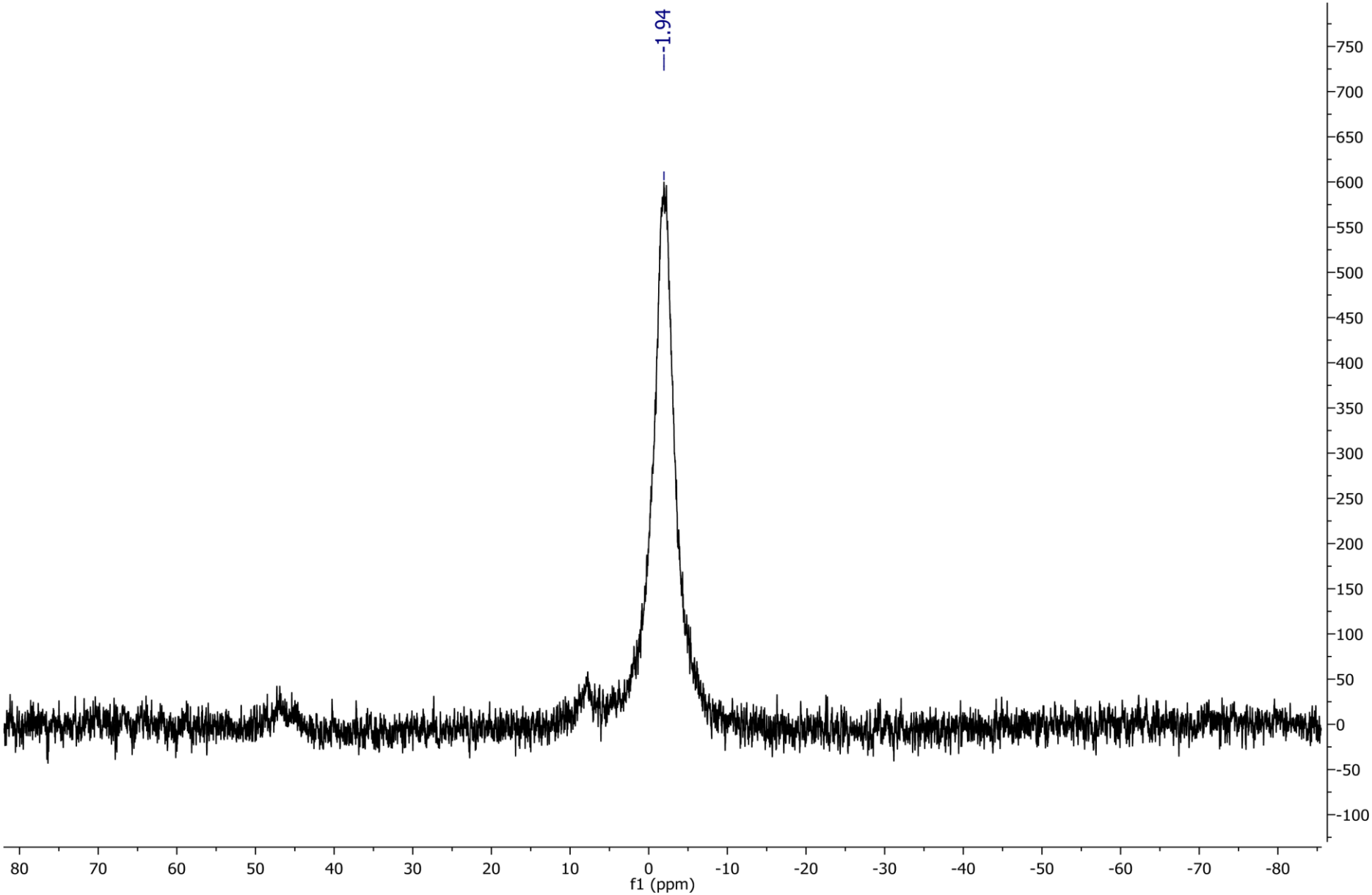

Figure S7. ^{11}B {^{1}H} NMR spectrum (160 MHz, benzene-*d*6) of **2**.

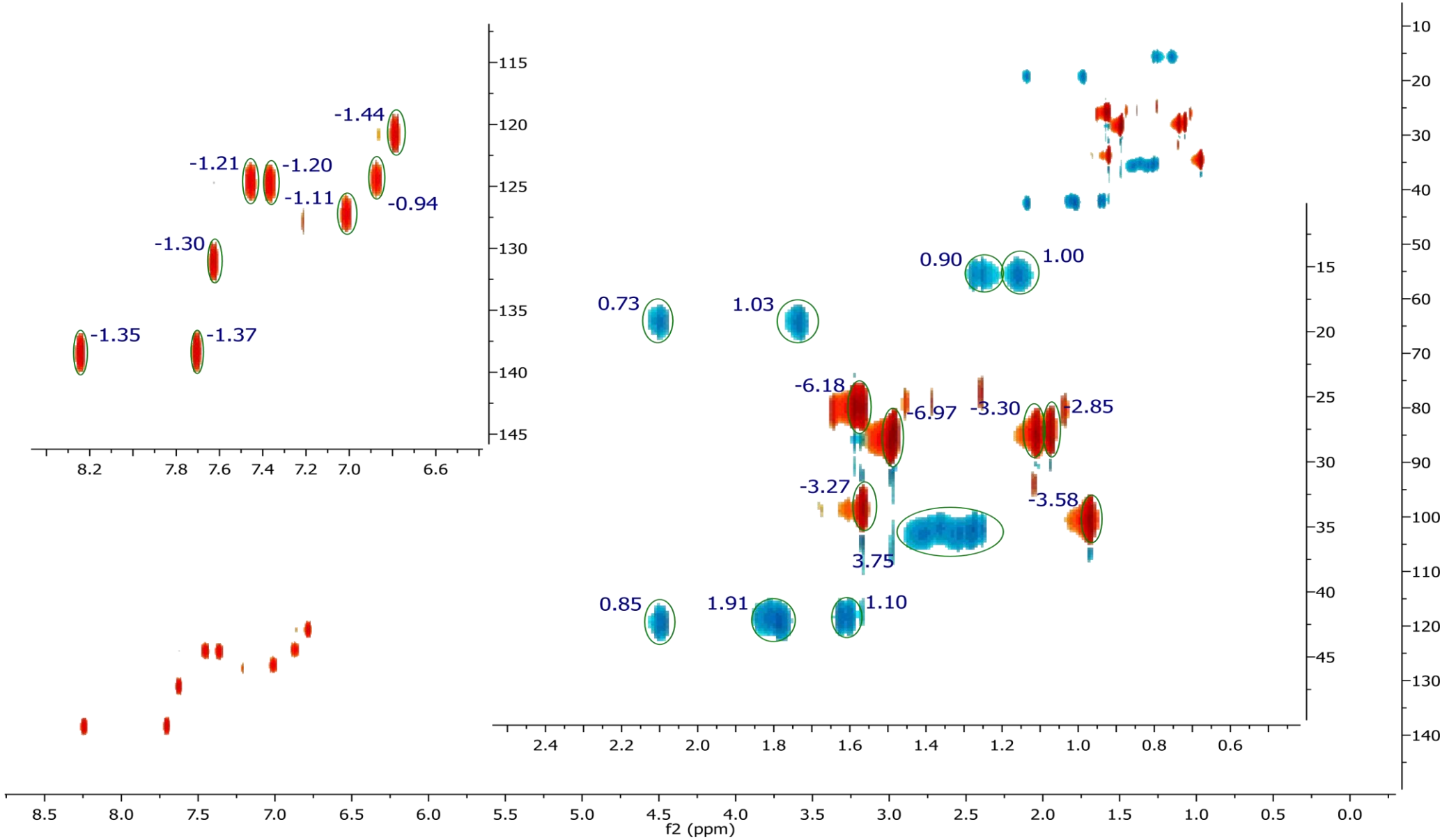

Figure S8. ^{13}C-^{1}H HSQC NMR spectrum (126 MHz–500 MHz, benzene-d_6) of **2**.

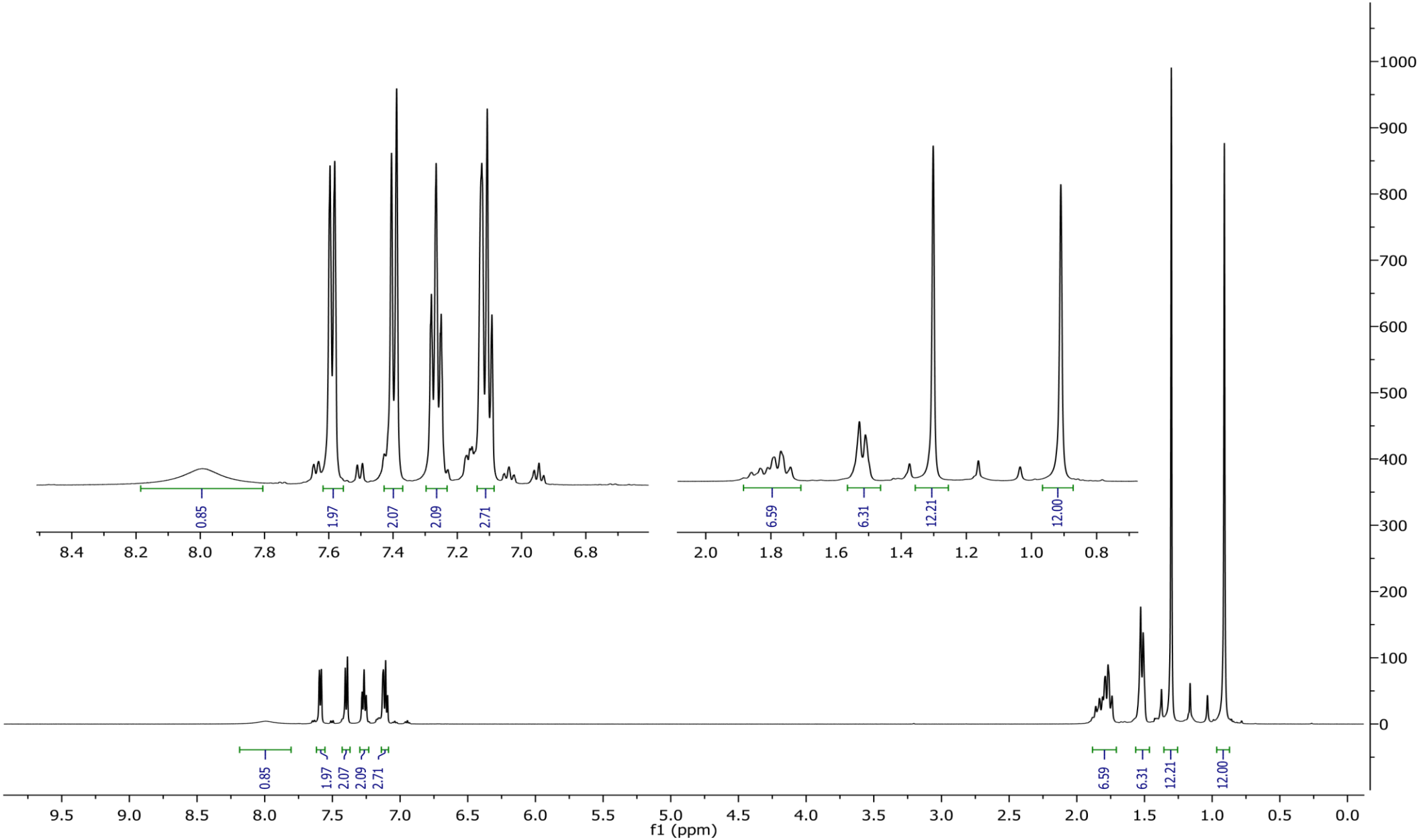

Figure S9. [1] H-NMR spectrum (500 MHz, benzene-d_6) of **3**.

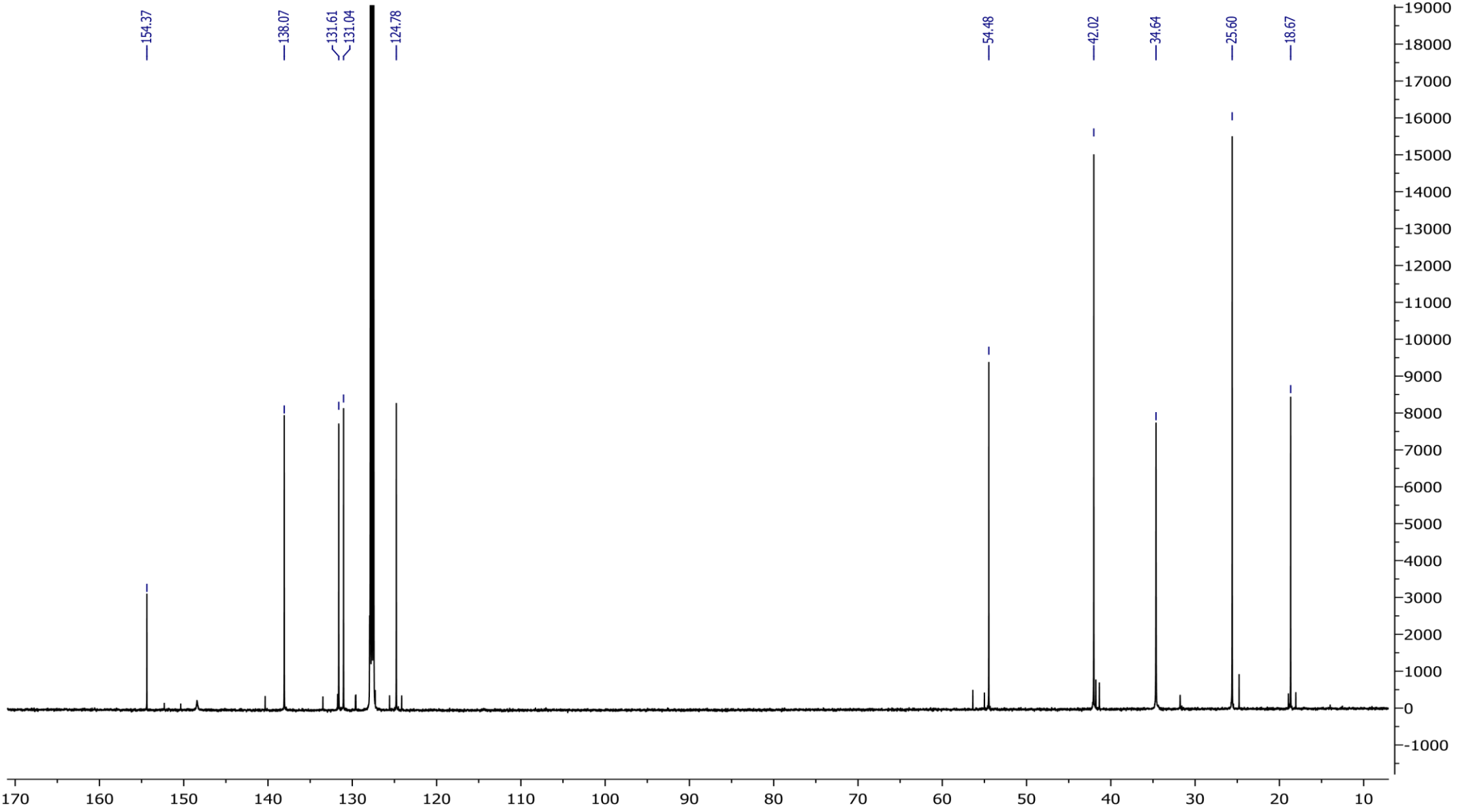

Figure S10. ^{13}C {^{1}H} NMR spectrum (126 MHz, benzene-*d*6) of **3**.

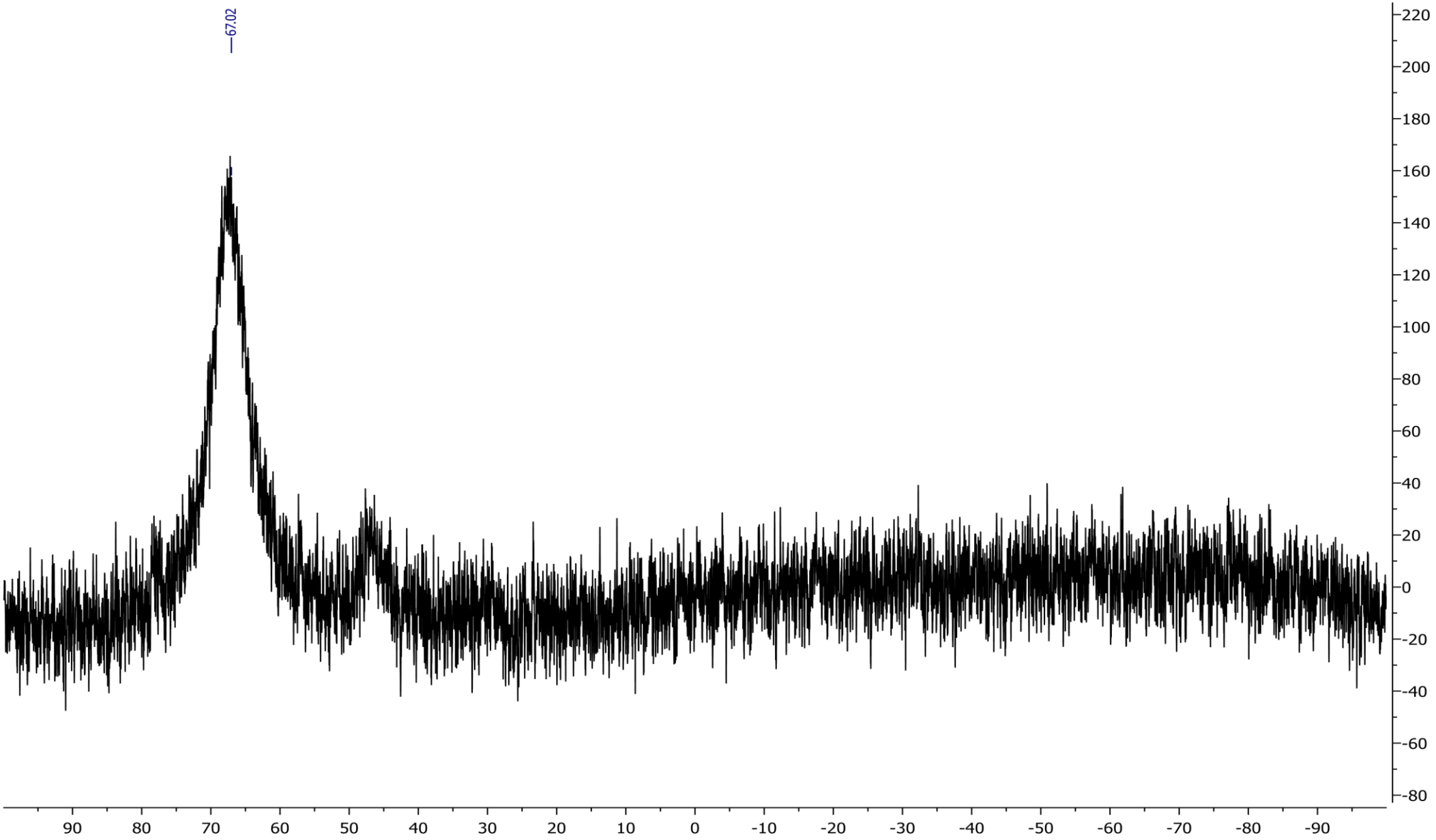

Figure S11. ^{11}B {^{1}H} NMR spectrum (160 MHz, benzene-*d*6) of **3**.

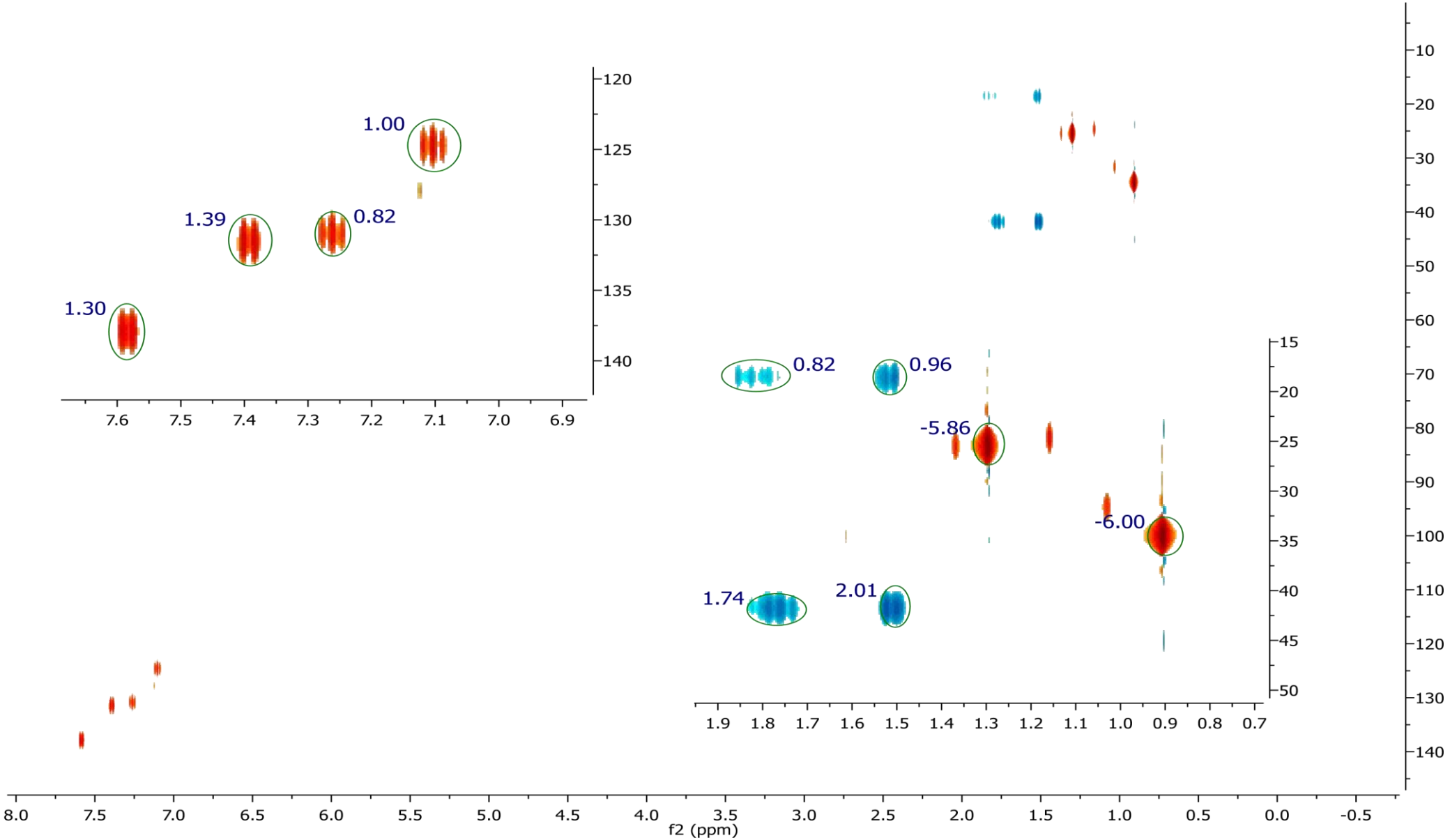

Figure S12. ^{13}C-^{1}H HSQC NMR spectrum (126 MHz–500 MHz, benzene-d_6) of **3**.

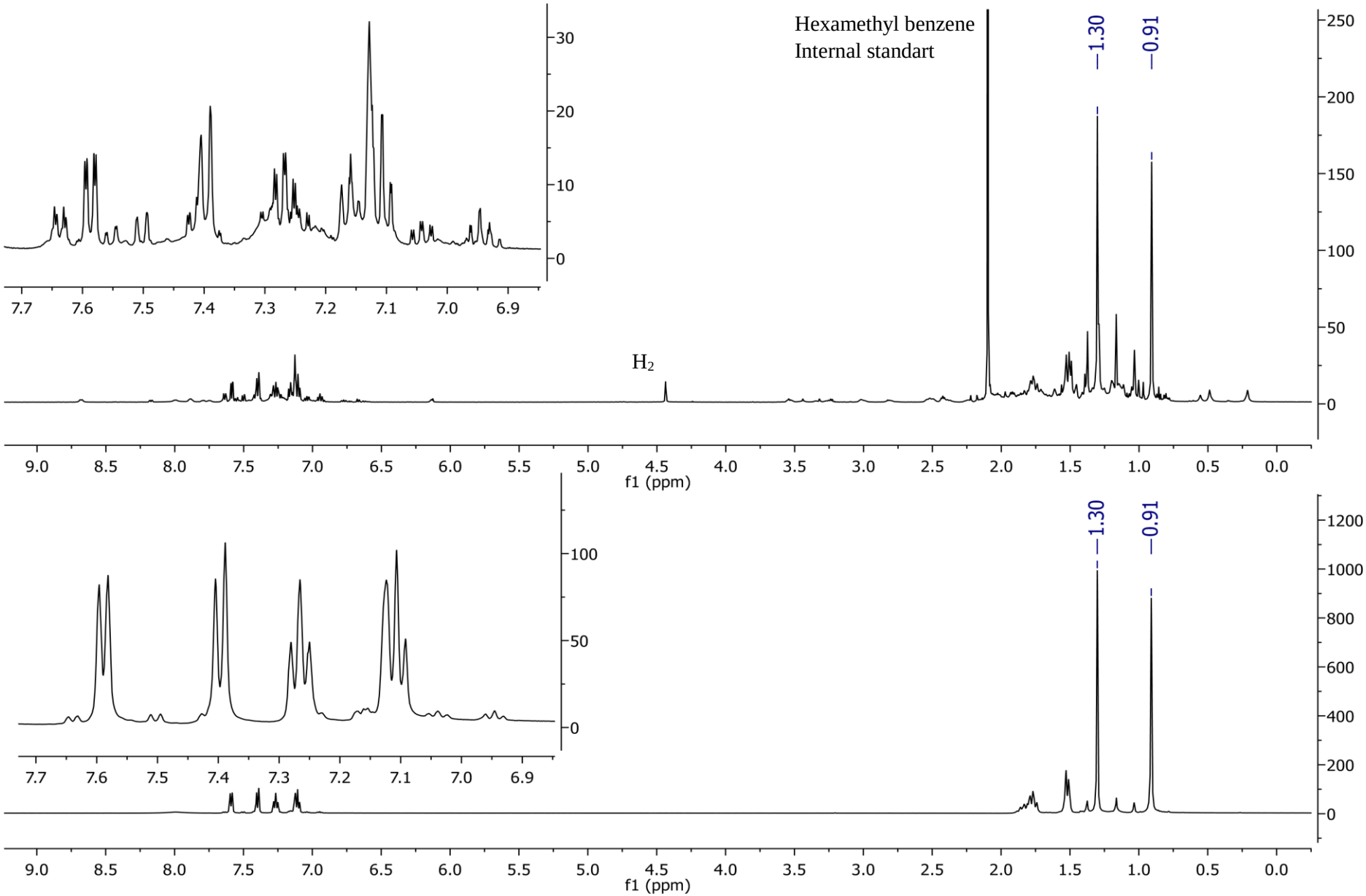

Figure S13: Top- Spectrum of **3** generated from the reaction of **2** with guanidine base TBD. Bottom- Spectra of **3**

Crystallographic data

Table S1. Crystal data and structure refinement for compounds **1-3**

	1	**2**	**3**
Empirical formula	C30 H44 B Cl N2	C30 H46 B Cl N2	C30 H45 B N2
Formula weight	478.93	480.95	445.49
Temperature	150(2) K	150(2) K	150(2) K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Orthorhombic	Monoclinic	Orthorhombic
Space group	Pccn	P 2_1/c	Pccn
Unit cell dimensions	a = 23.1183(12) Å b = 7.8422(4) Å c = 15.1217(8) Å α= β= γ = 90°.	a = 18.4751(11) Å b = 9.3581(5) Å c = 19.2220(11) Å α= γ = 90°. β= 111.6810(10)°.	a = 22.4146(12) Å b = 7.7550(4) Å c = 15.5401(8) Å α= β= γ = 90°.
Volume	2741.5(2) $Å^3$	3088.2(3) $Å^3$	2701.3(2) $Å^3$
Z	4	4	4
Density (calculated)	1.160 Mg/m^3	1.034 Mg/m^3	1.095 Mg/m^3
Absorption coefficient	0.160 mm^{-1}	0.142 mm^{-1}	0.062 mm^{-1}
F(000)	1040	1048	980
Crystal size	0.62 x 0.54 x 0.26 mm^3	0.42 x 0.28 x 0.20 mm^3	0.38 x 0.28 x 0.12 mm^3
Theta range for data collection	1.762 to 28.260°.	2.147 to 26.373°.	1.817 to 28.270°.
Index ranges	-30<=h<=30, -10<=k<=10, -20<=l<=20	-23<=h<=,23 -11<=k<=11, -24<=l<=23	-29<=h<=29, -10<=k<=10, -20<=l<=20
Reflections collected	28520	29413	25531
Independent reflections	3406 [R(int) = 0.0293]	6312 [R(int) = 0.0302]	3356 [R(int) = 0.0327]

Completeness to theta = 25.242°	100.0 %	100.0 %	100.0%
Max. and min. transmission	0.959 and 0.906	0.7454 and 0.7039	0.977 and 0.993
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	3406 / 0 / 159	6312/0/323	3356 / 0 / 158
Goodness-of-fit on F^2	1.029	1.039	1.026
Final R indices [I>2sigma(I)]	R1 = 0.0405, wR2 = 0.1064	R1 = 0.0389, wR2 = 0.0925	R1 = 0.0476, wR2 = 0.1171
R indices (all data)	R1 = 0.0481, wR2 = 0.1129	R1 = 0.0530, wR2 = 0.0982	R1 = 0.0593, wR2 = 0.1261
Largest diff. peak and hole	0.362 and -0.516 e.$Å^{-3}$	0.241 and -0.189 e.$Å^{-3}$	0.373, and -0.156 e.$Å^{-3}$