Supporting Information for:

Probing the Reactivity of Pentaphenylborole with N-H, O-H, P-H, and S-H Bonds

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Figure S-1: Stacked plot of crude ^{1}H NMR spectra of the reaction of **A** with H_2O (top) and isolated **12** (bottom) in $CDCl_3$ († CH_2Cl_2, * hexanes, • $CDCl_3$).

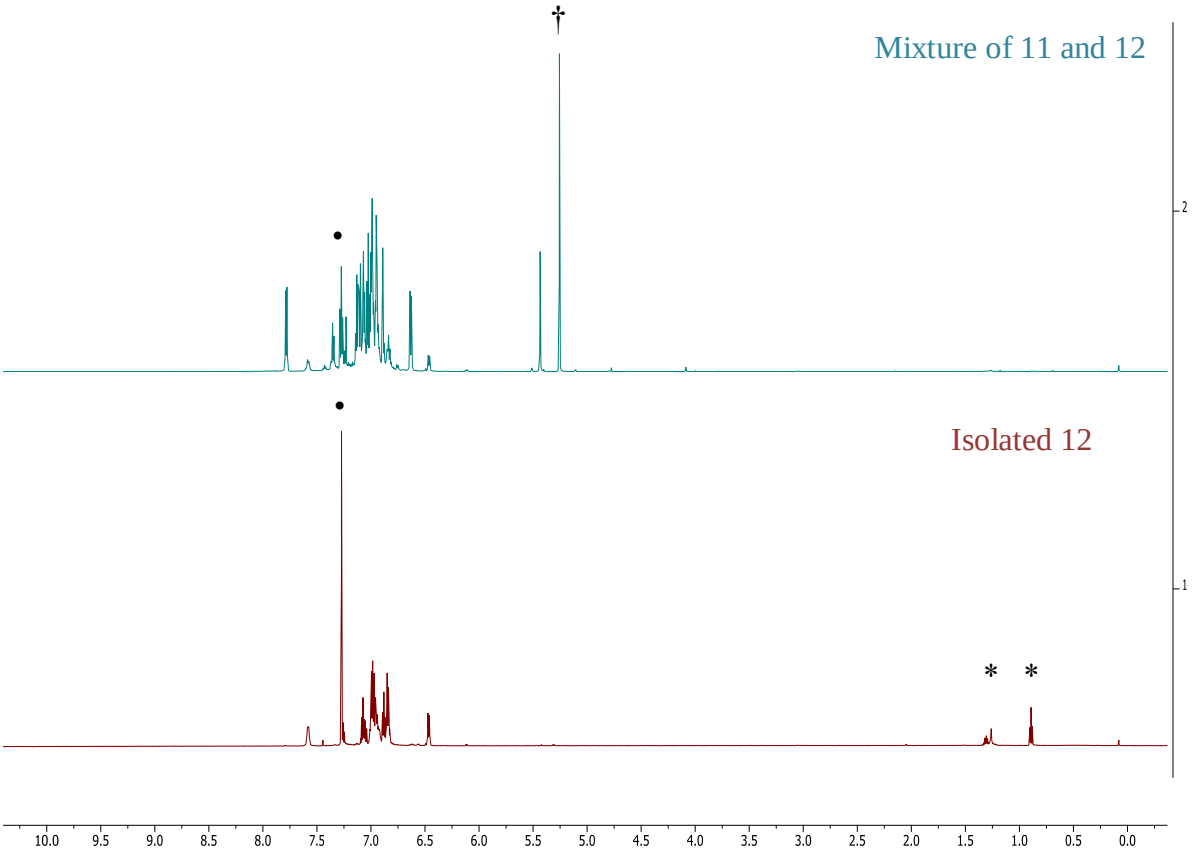


Figure S-2: FT-IR spectrum of crude reaction of **A** with H_2O.

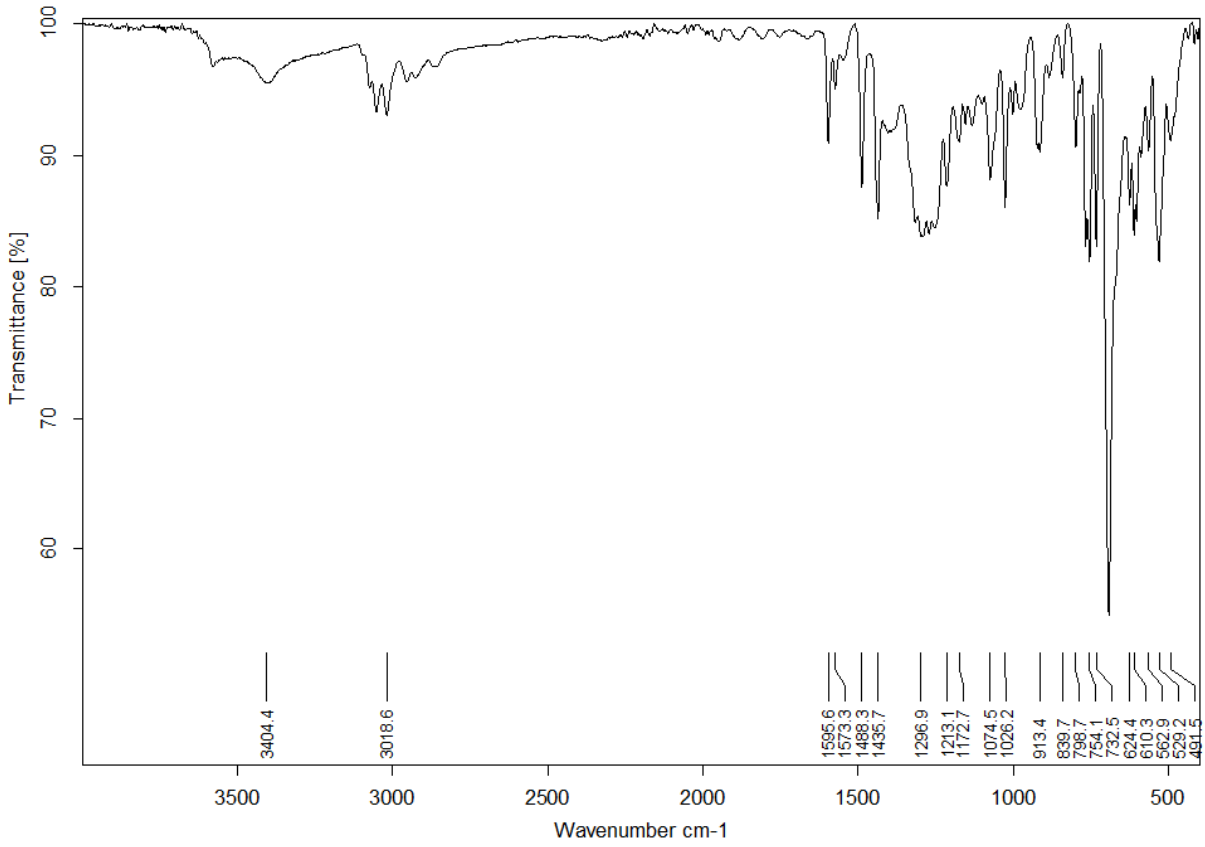


Figure S-3: ^{1}H NMR spectrum of **12** in $CDCl_3$ (*hexanes).

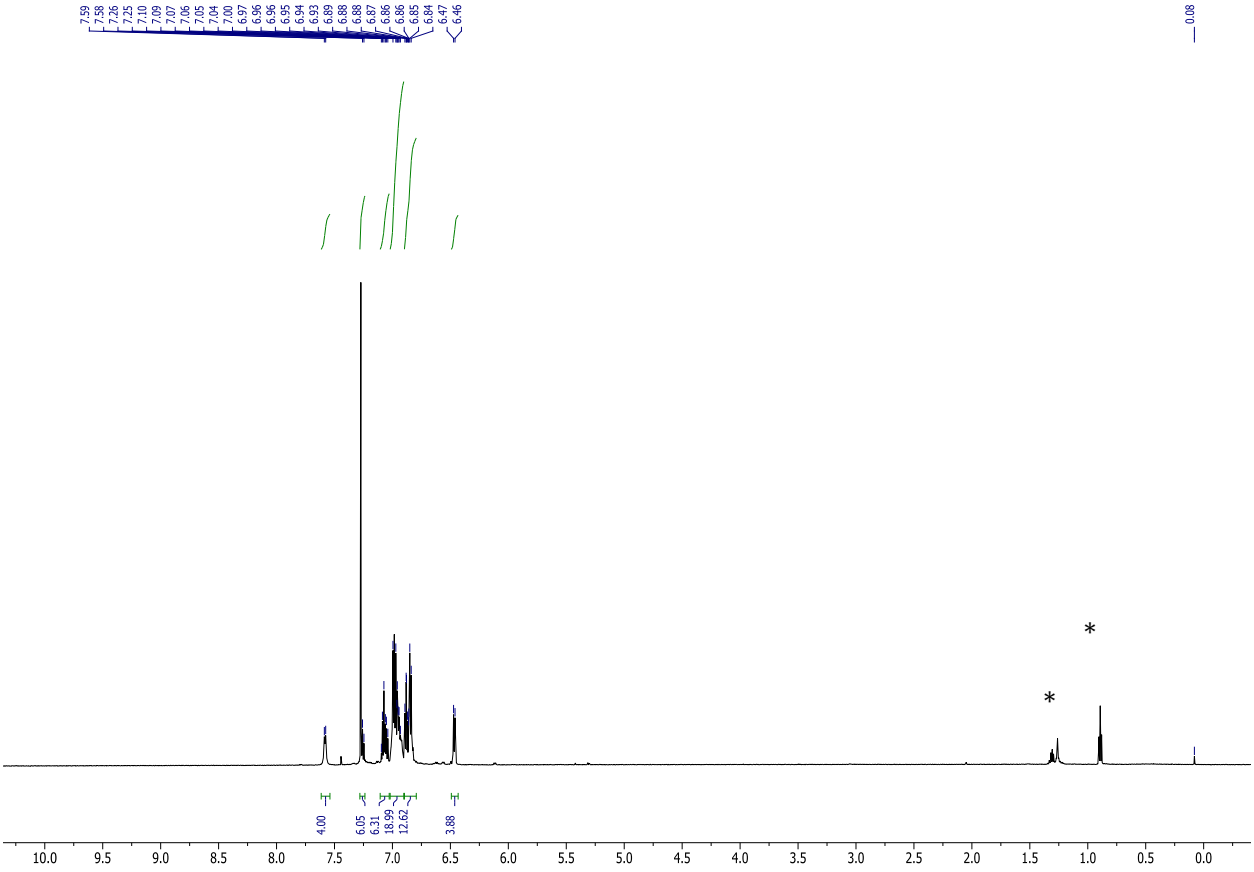


Figure S-4: Expansion of aromatic region of ^{1}H NMR spectrum of **12** in $CDCl_3$.

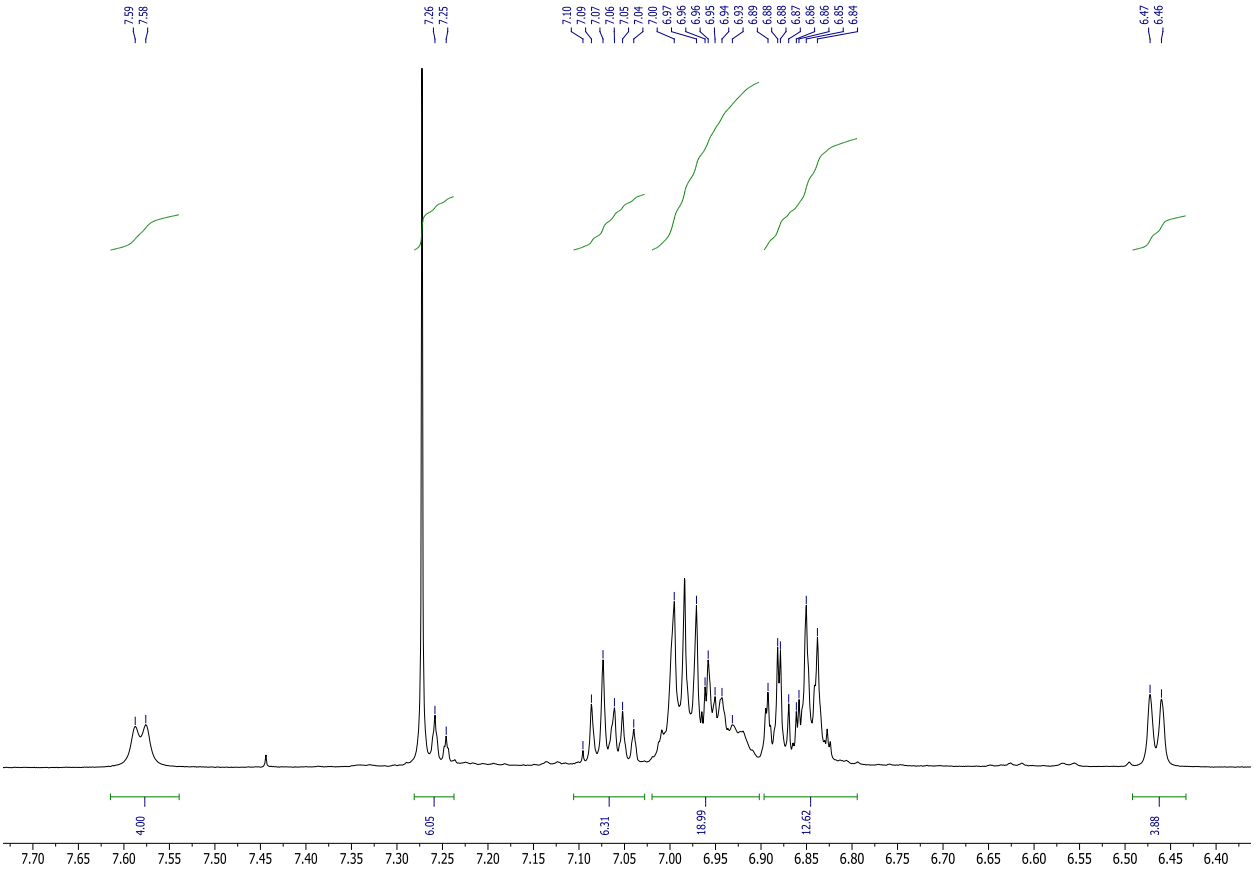


Figure S-5: $^{11}B\{^{1}H\}$ NMR spectrum of **12** in $CDCl_3$.

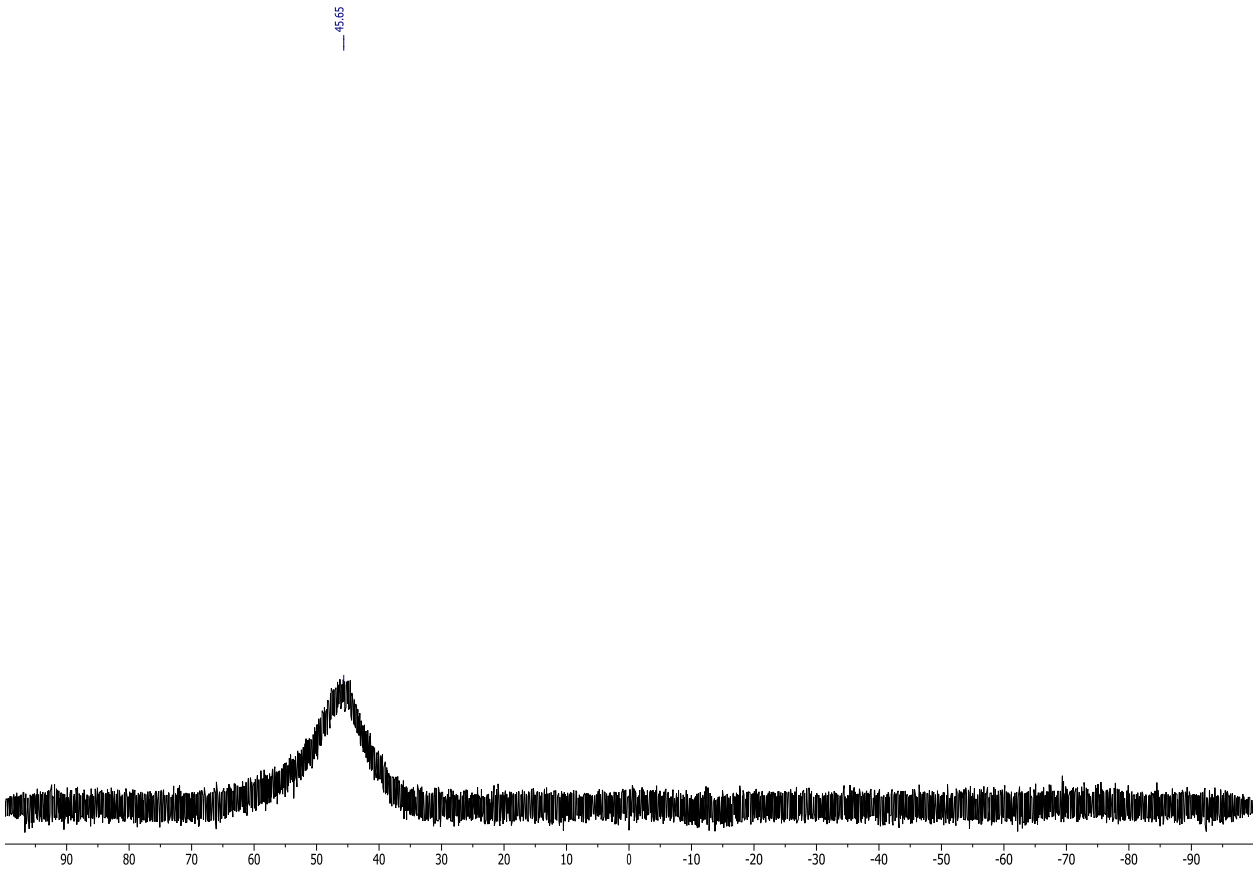


Figure S-6: $^{13}C\{^{1}H\}$ NMR spectrum of **12** in $CDCl_3$ (*hexanes).

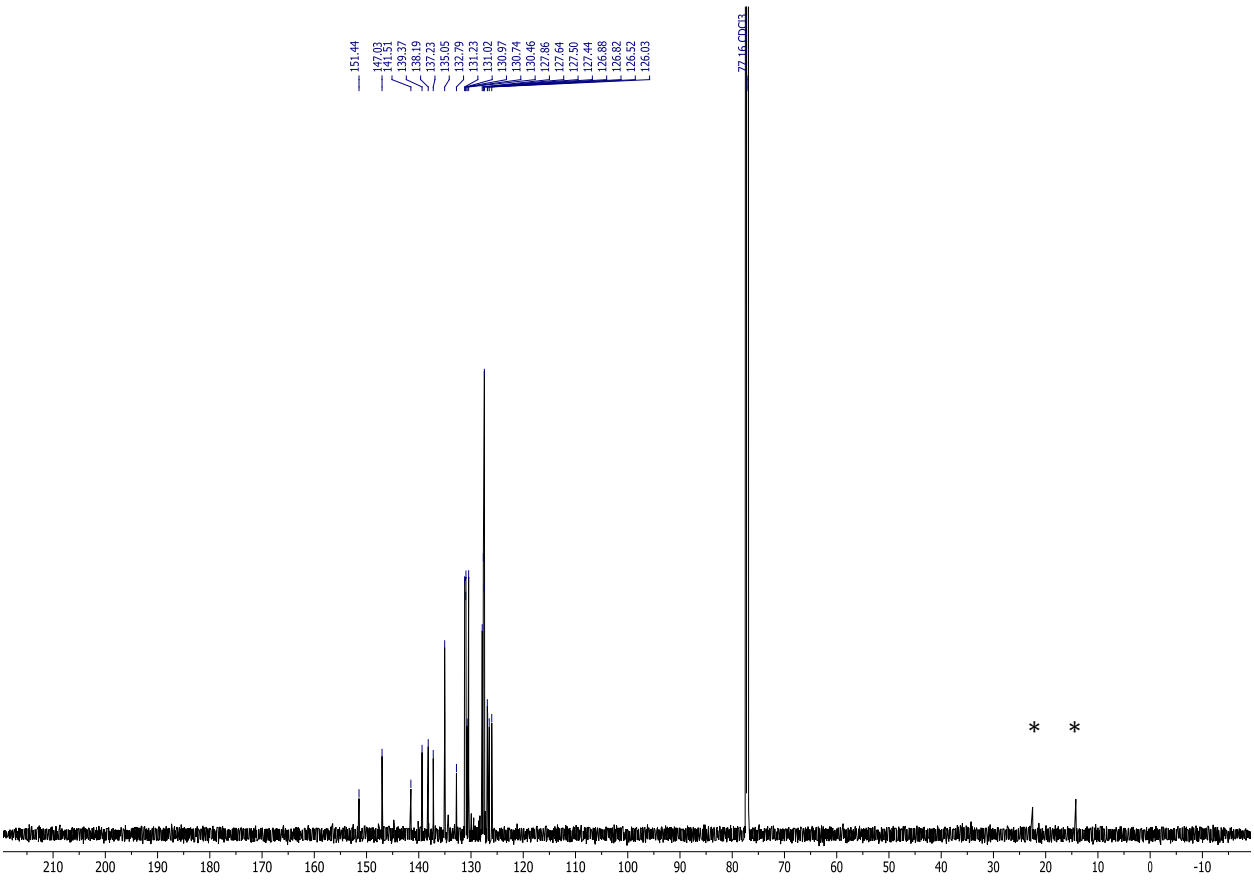


Figure S-7: Expansion of $^{13}C\{^{1}H\}$ NMR spectrum of **12** in $CDCl_3$.

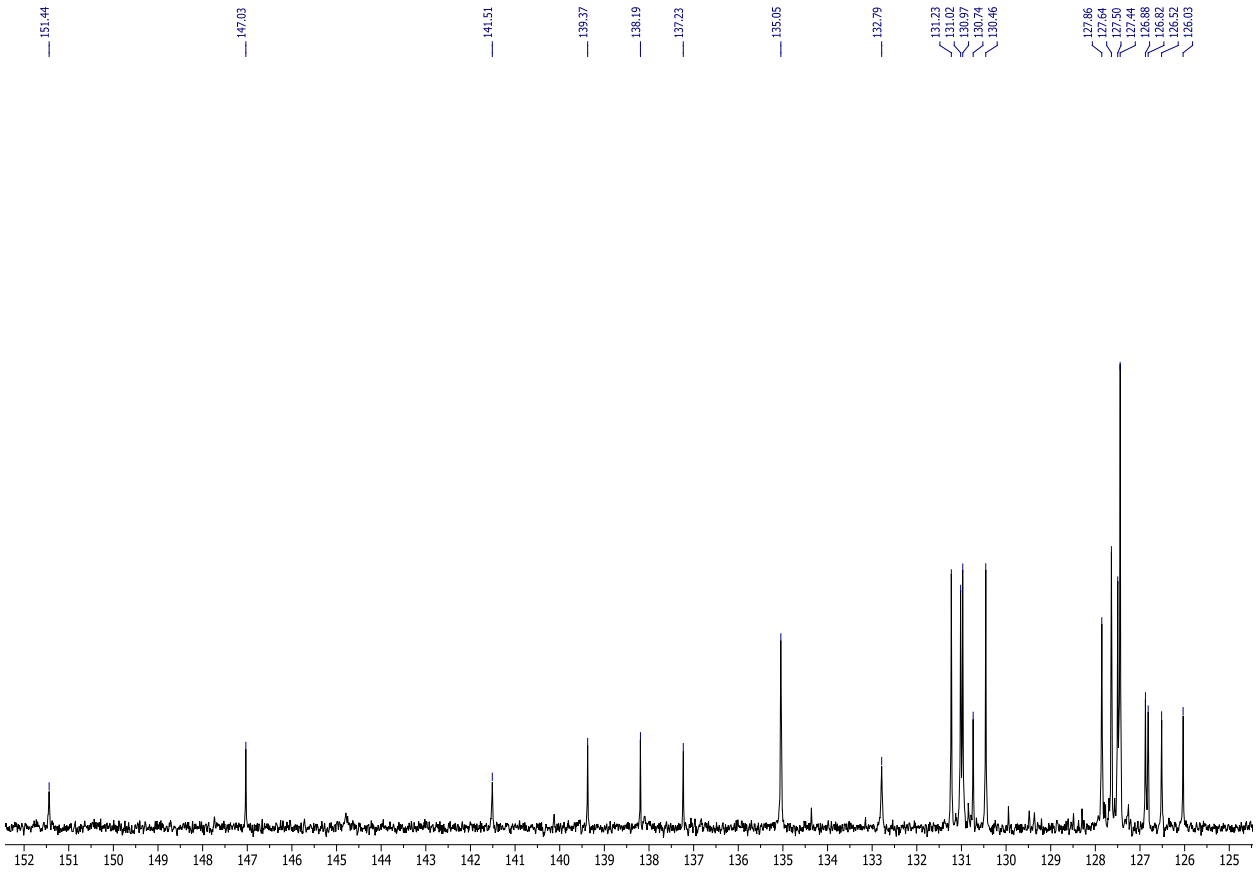


Figure S-8: FT-IR spectrum of **12**.

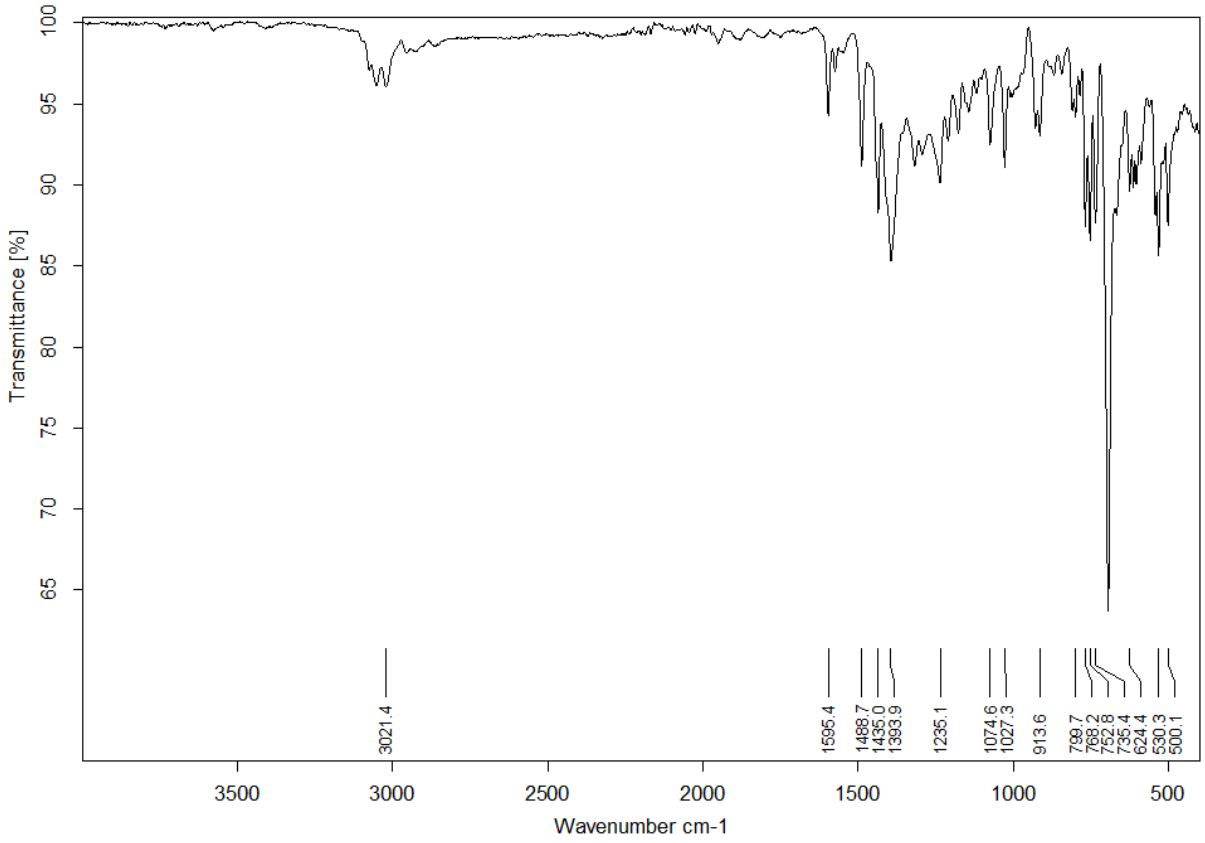


Figure S-9: ^{1}H NMR of **13** at 25˚C and -30˚C in $CDCl_3$.

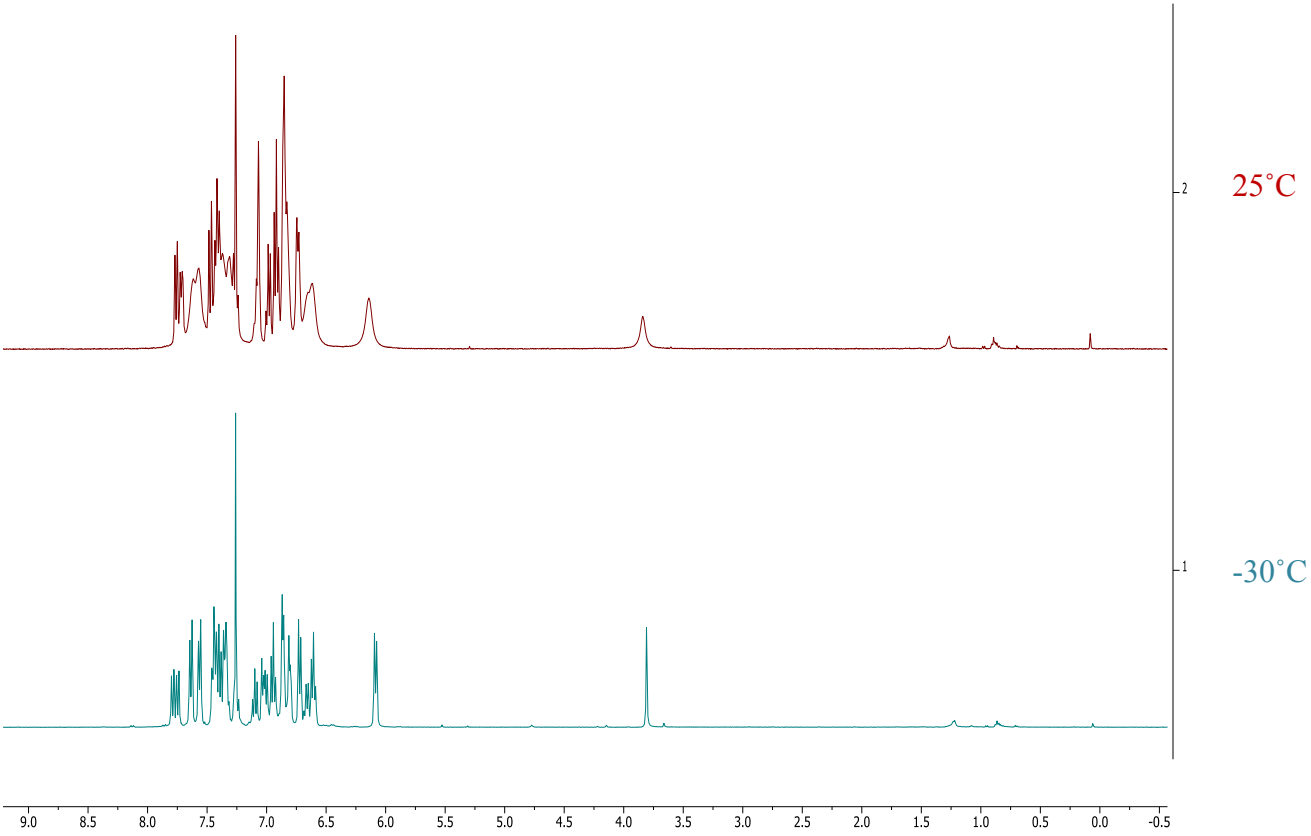


Figure S-10: ^{1}H NMR spectrum of **13** in $CDCl_3$ at -30˚C (*hexanes).

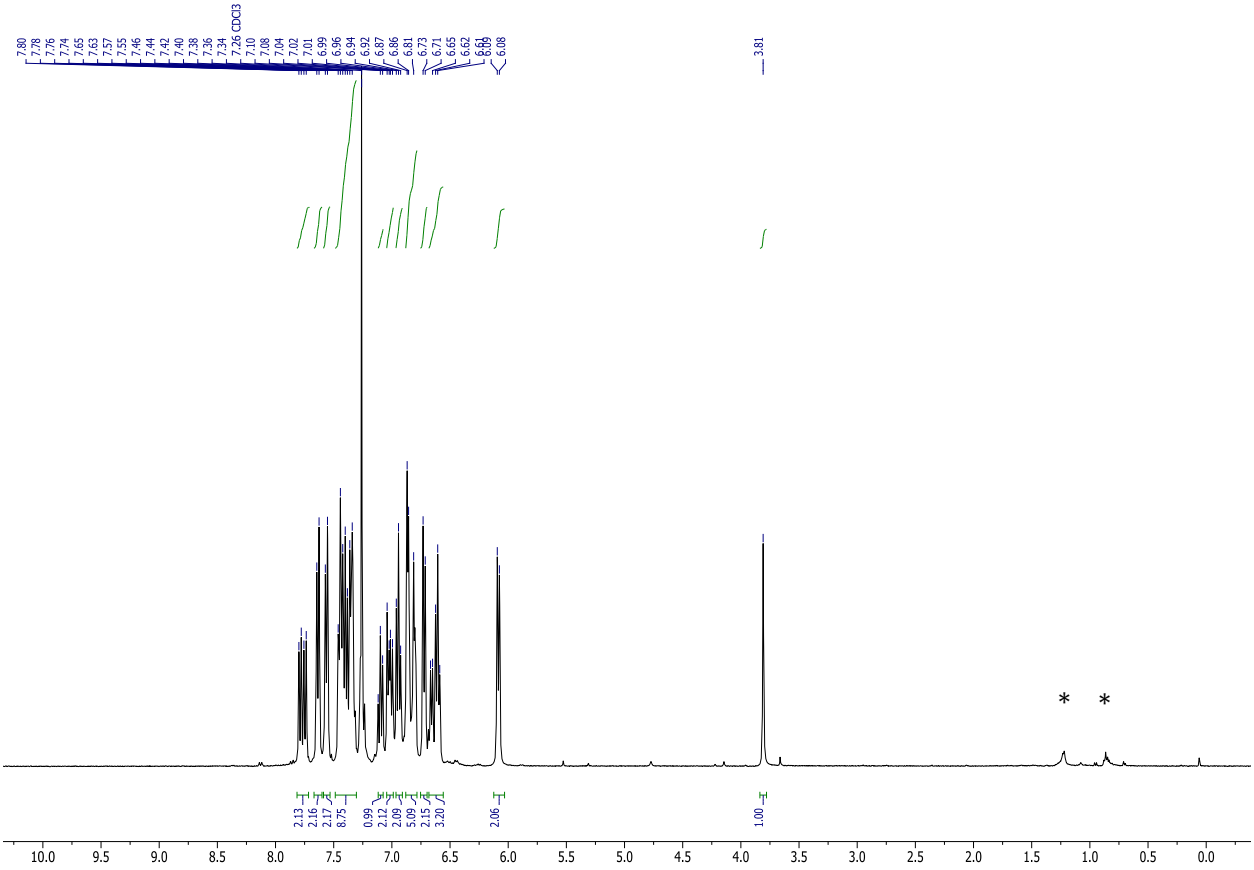


Figure S-11: Expansion of ^{1}H NMR spectrum of **13** in $CDCl_3$ at -30˚C.

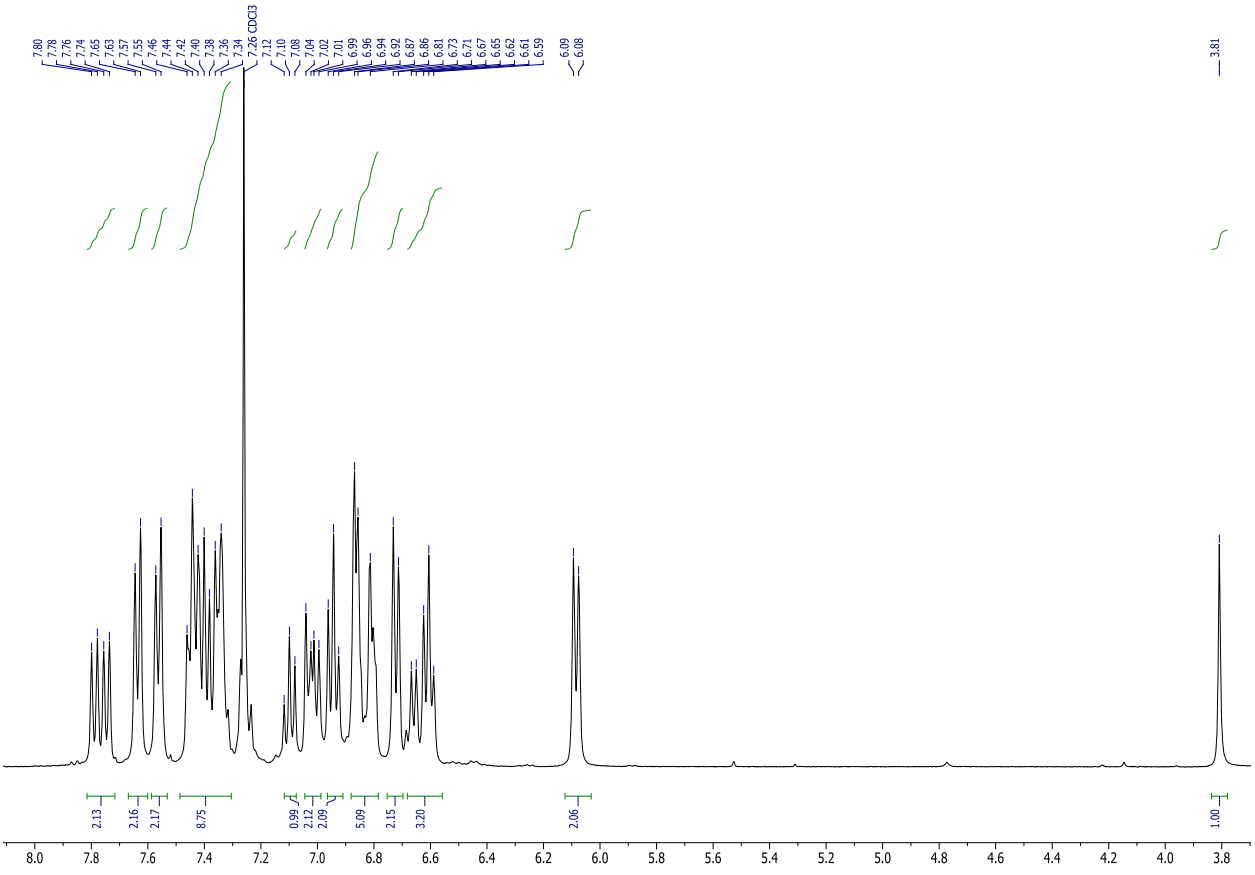


Figure S-12: $^{11}B\{^{1}H\}$ NMR spectrum of **13** in $CDCl_3$ at -30˚C.

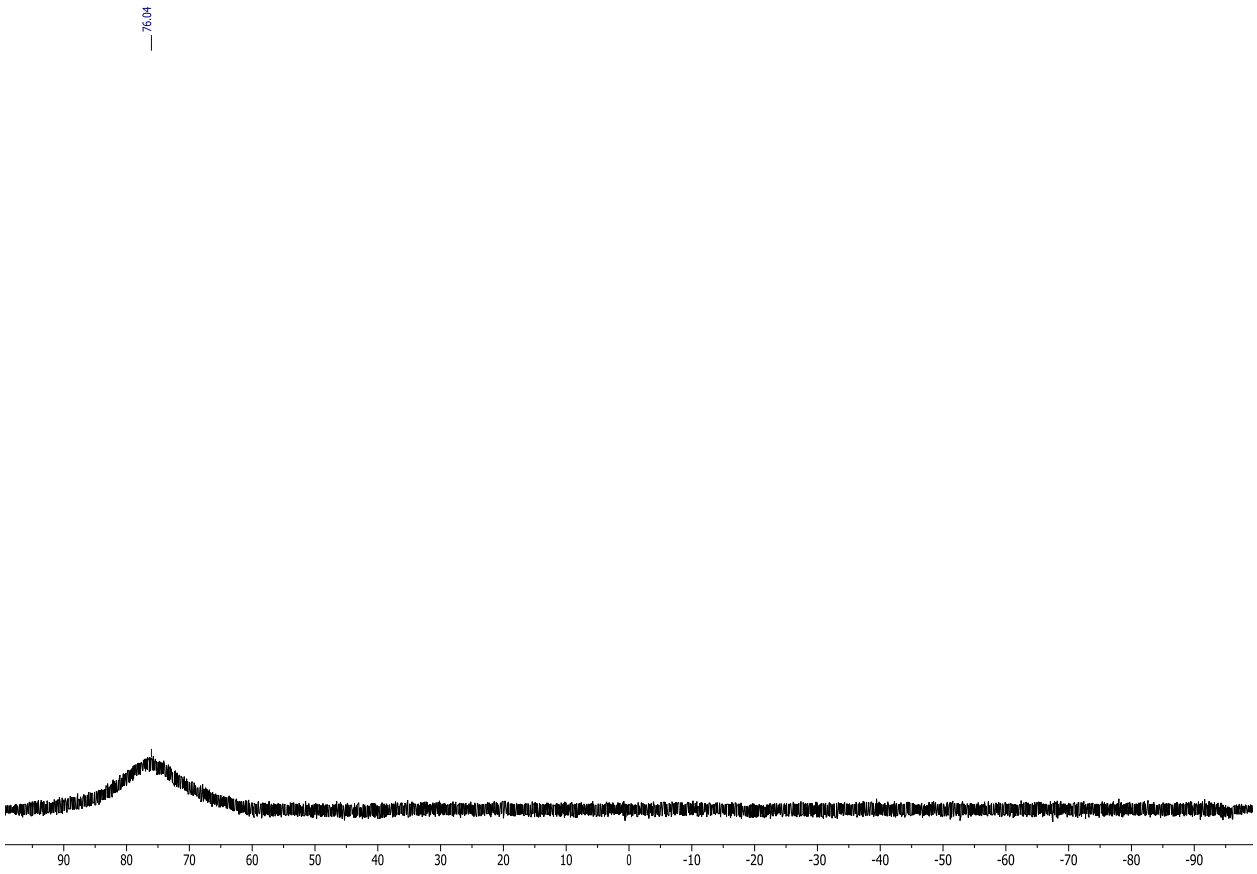


Figure S-13: $^{13}C\{^{1}H\}$NMR spectrum of **13** in $CDCl_3$ at -30˚C.

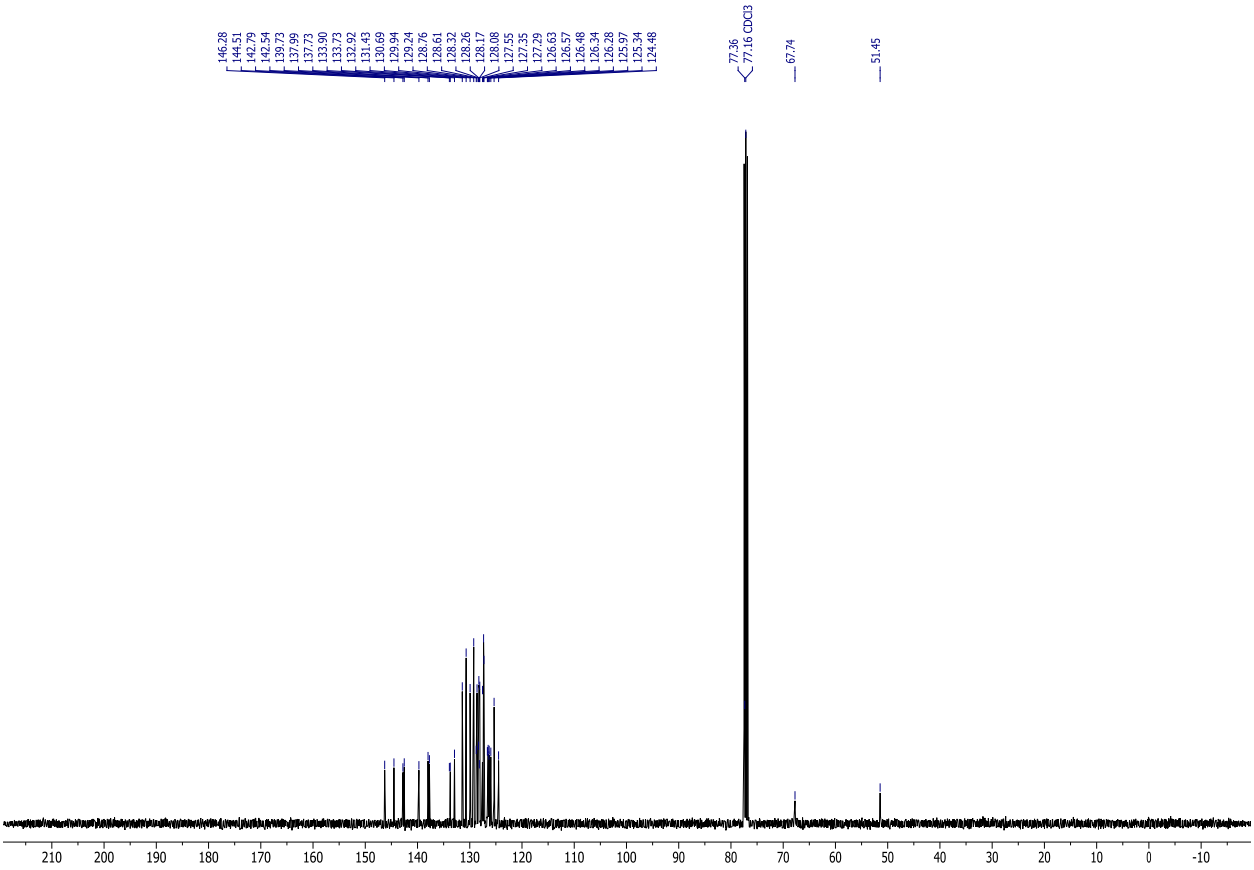


Figure S-14: Expansion of $^{13}C\{^{1}H\}$ NMR spectrum of **13** in $CDCl_3$ at -30˚C.

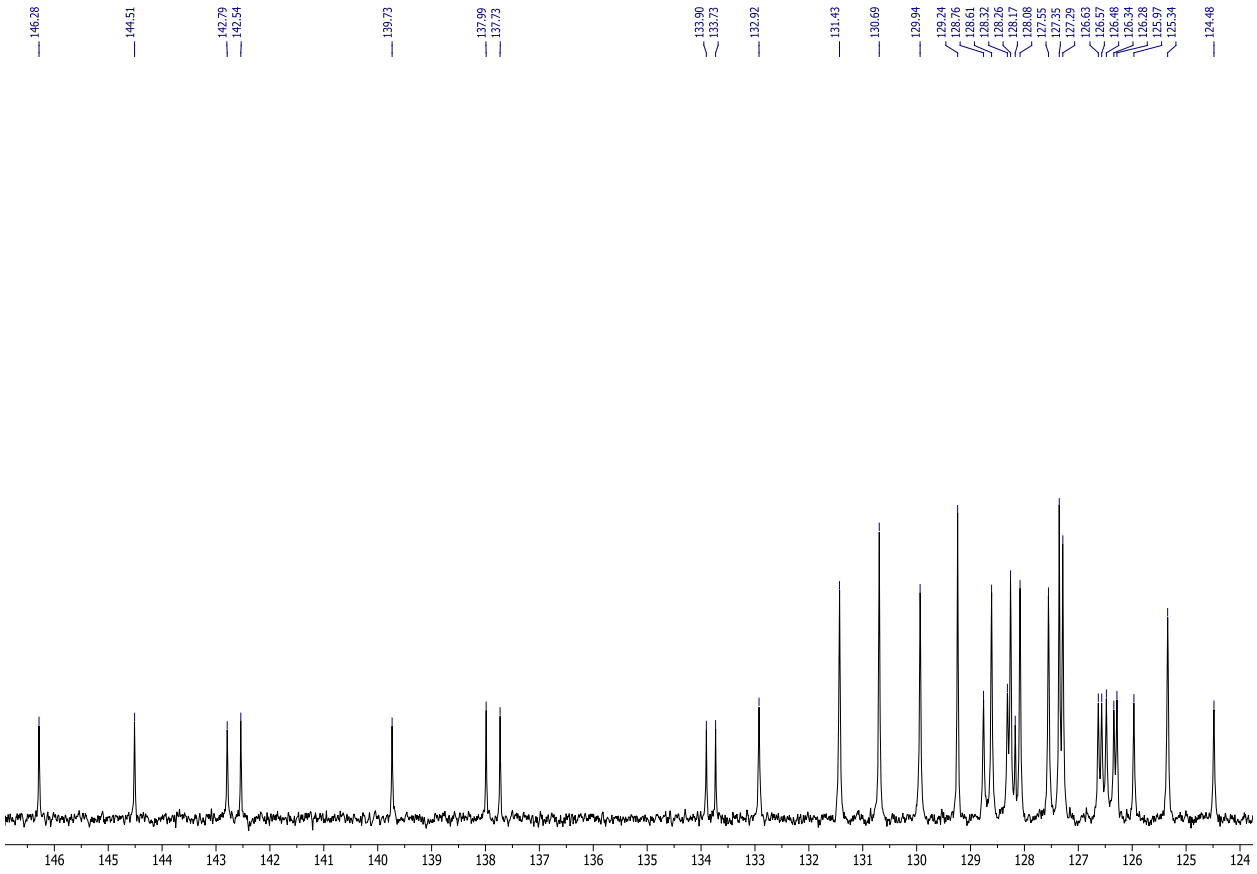


Figure S-15: FT-IR spectrum of **13**.

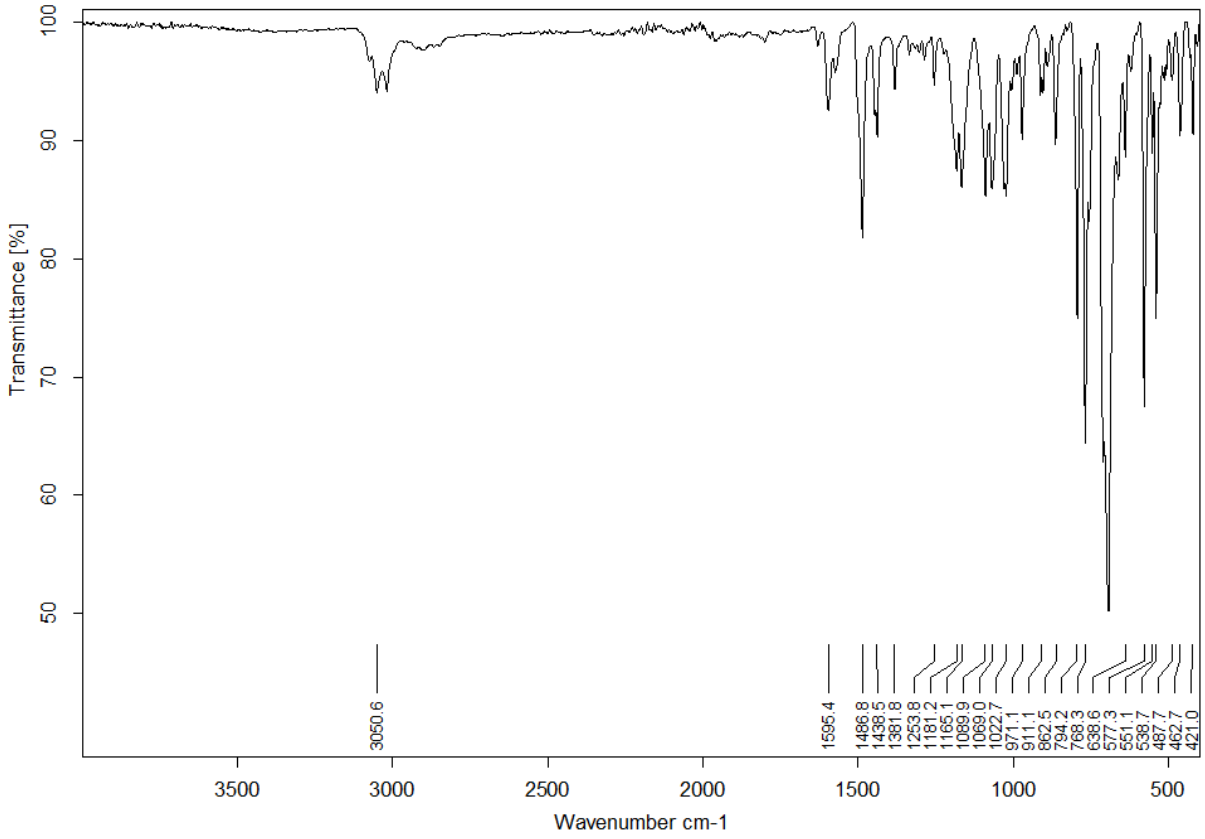


Figure S-16: ^{1}H NMR spectrum of **14** in $CDCl_3$ (*hexanes).

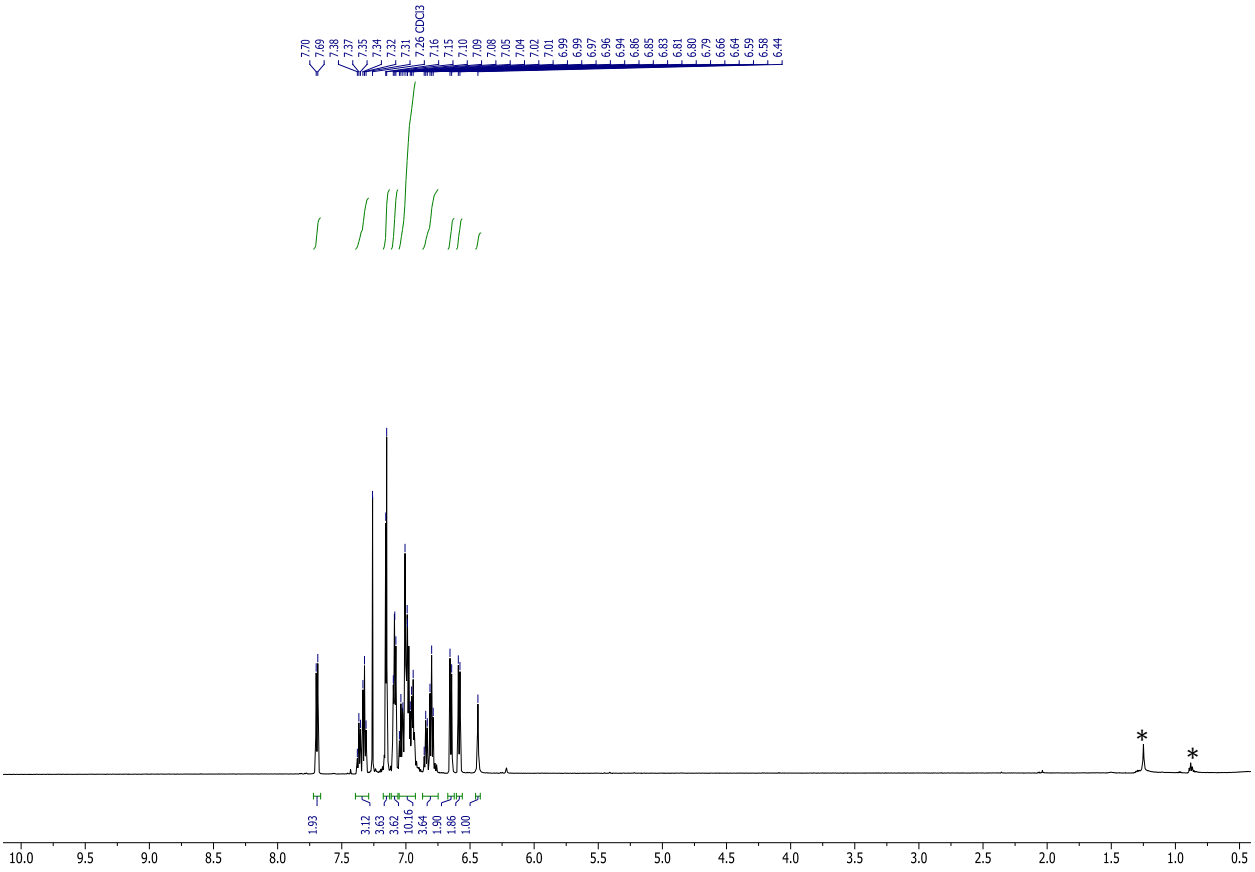


Figure S-17: Expansion of aromatic region of ^{1}H NMR spectrum of **14** in $CDCl_3$.

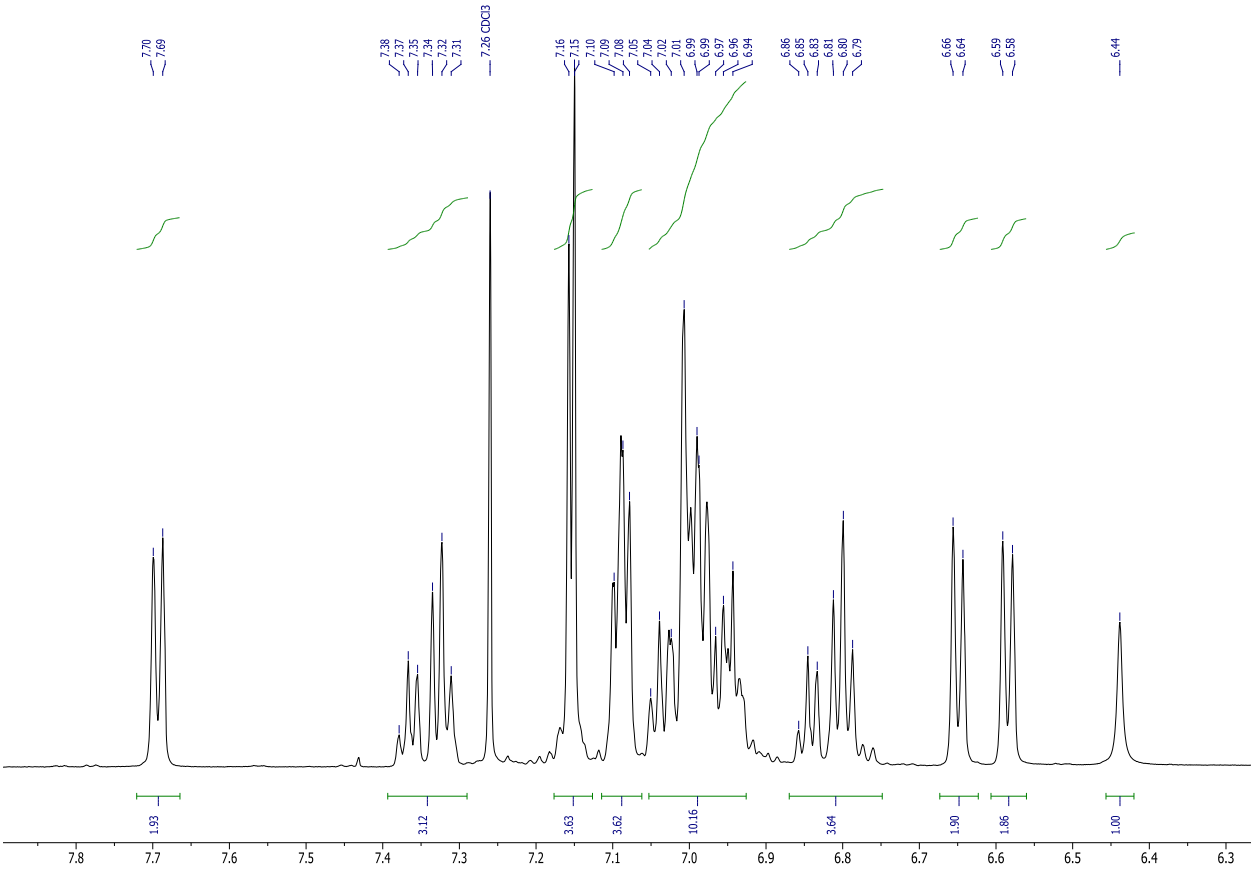


Figure S-18: $^{11}B\{^{1}H\}$ NMR spectrum of **14** in $CDCl_3$.

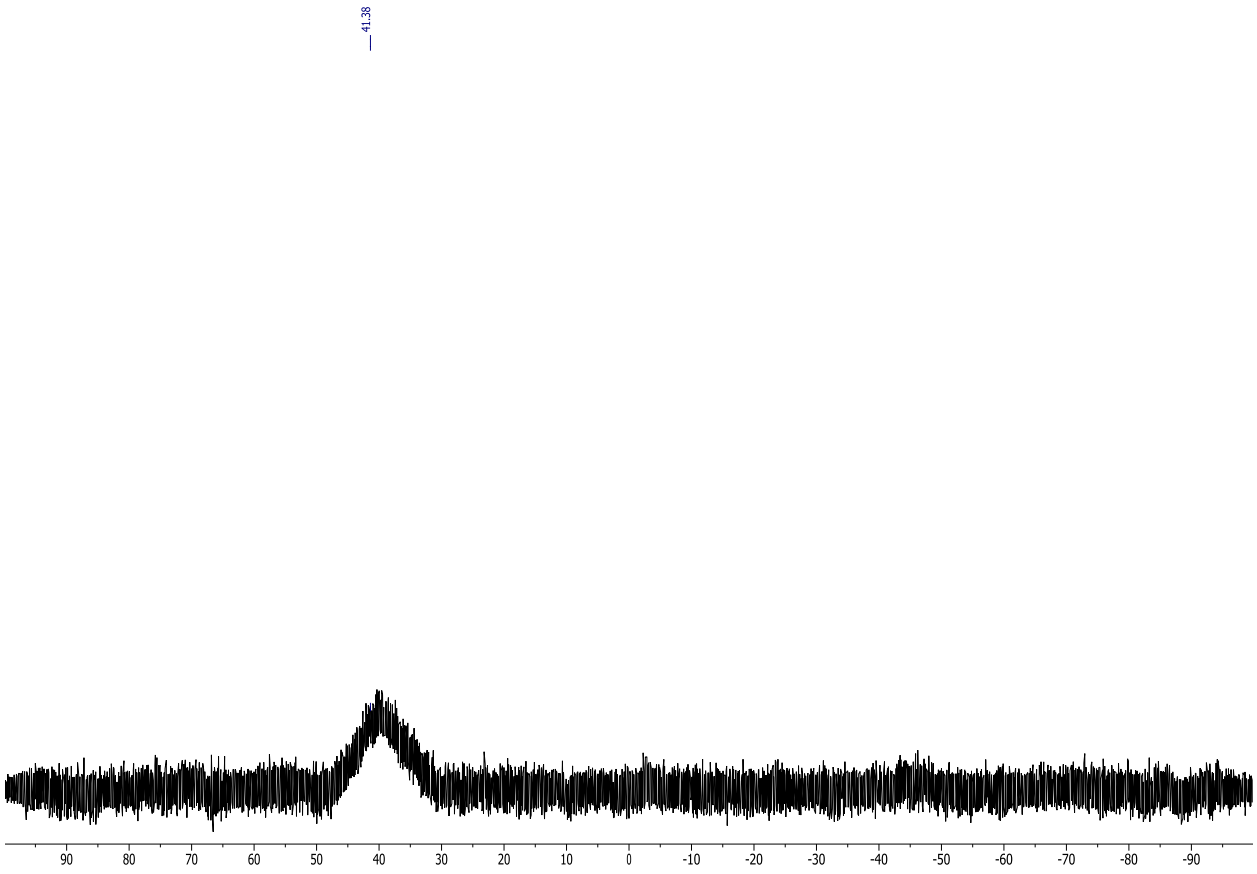


Figure S-19: $^{13}C\{^{1}H\}$ NMR spectrum of **14** in $CDCl_3$.

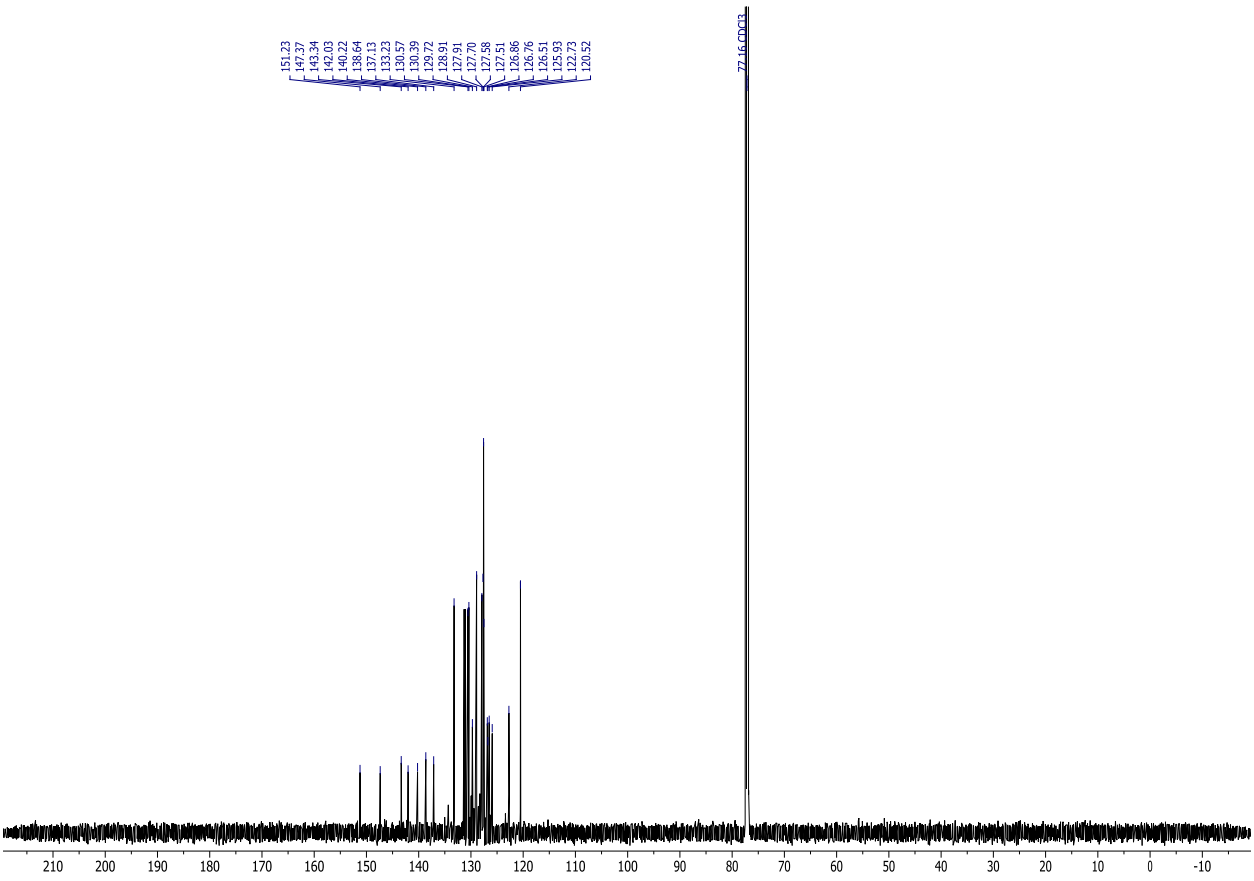


Figure S-20: Expansion of $^{13}C\{^{1}H\}$ NMR spectrum of **14** in $CDCl_3$.

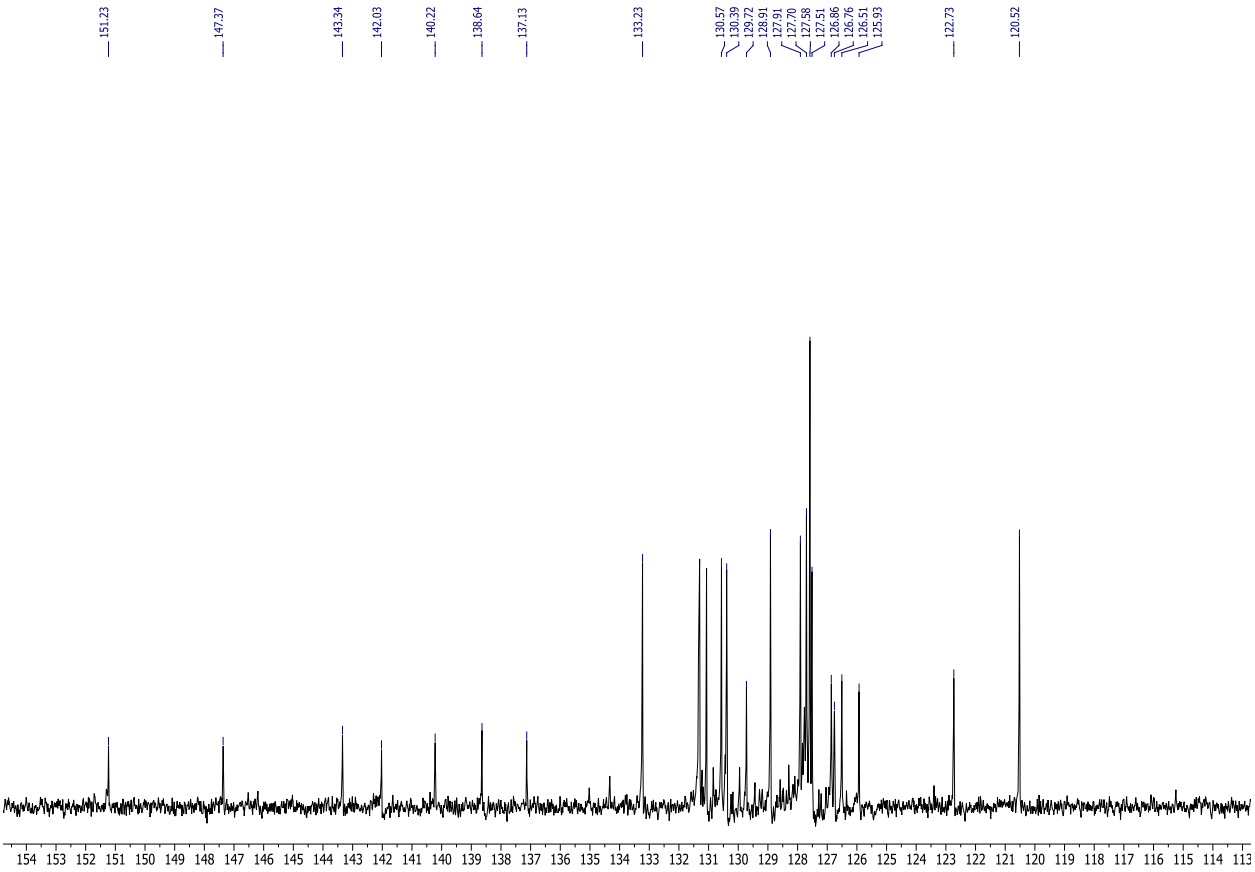


Figure S-21: Stacked plot of crude $^{11}B\{^{1}H\}$ NMR spectra of the reaction of **A** with aniline at -40˚C in $CDCl_3$ over a period of ten minutes.

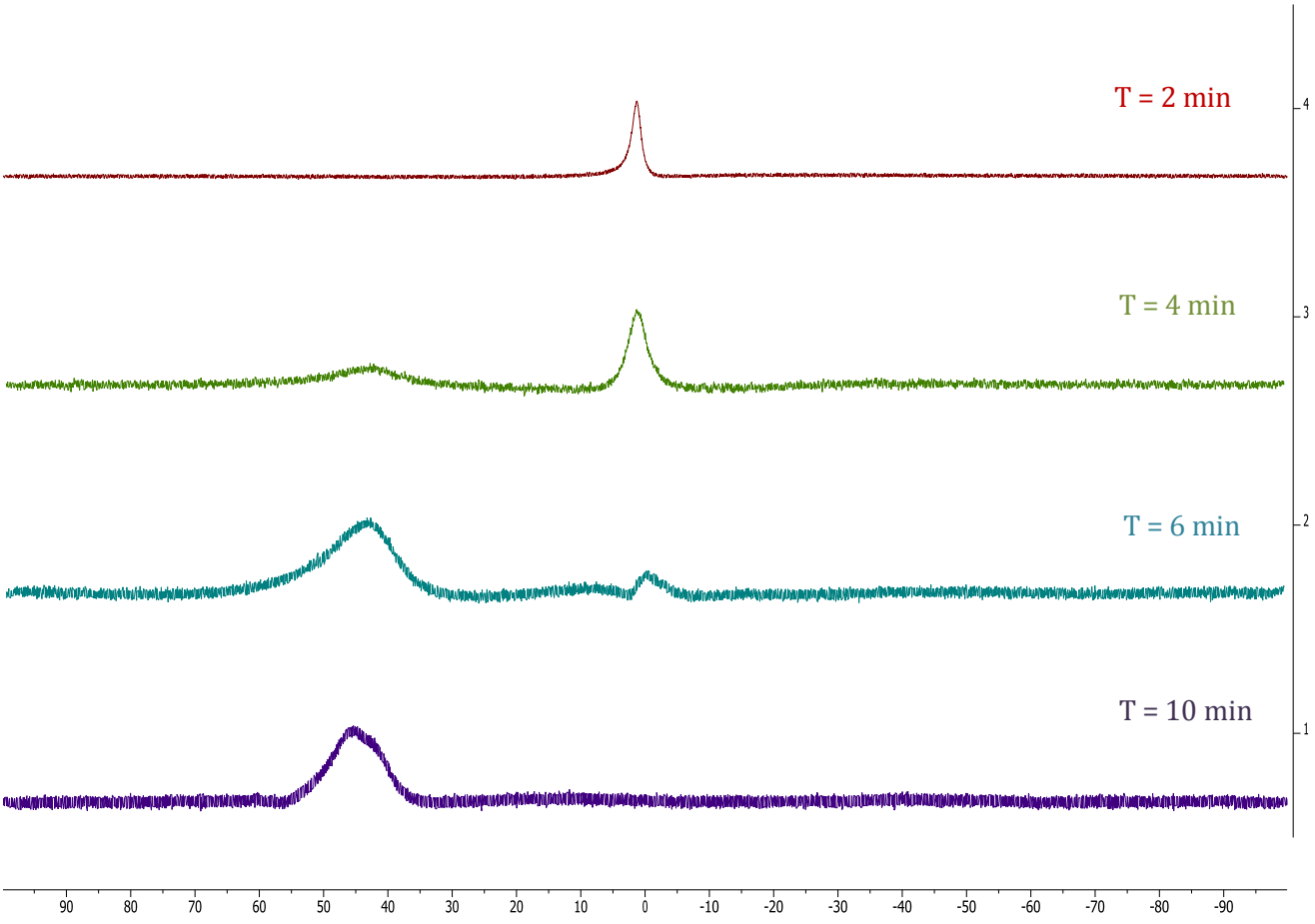


Figure S-22: FT-IR spectrum of **14**.

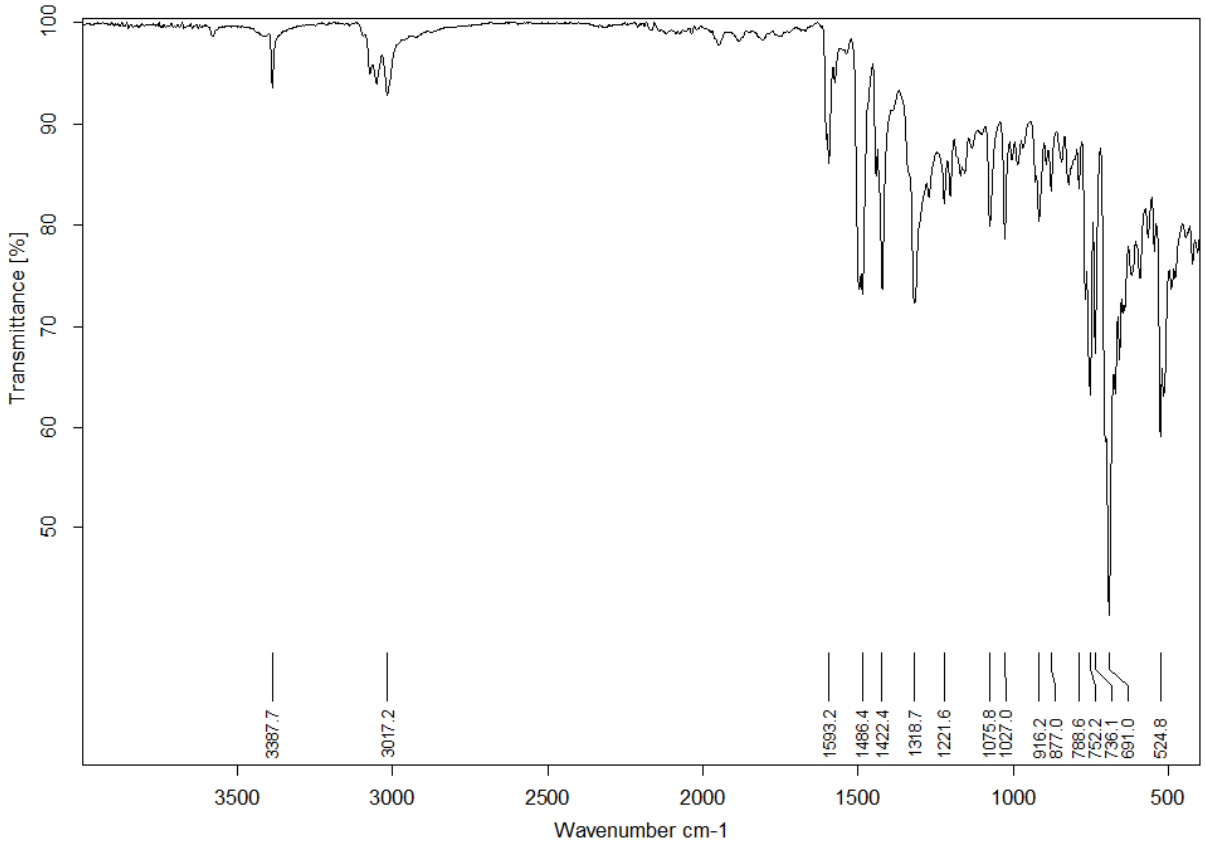


Figure S-23: ^{1}H NMR spectrum of **15** in $CDCl_3$ († CH_2Cl_2, * *n*-pentane, • silicone grease).

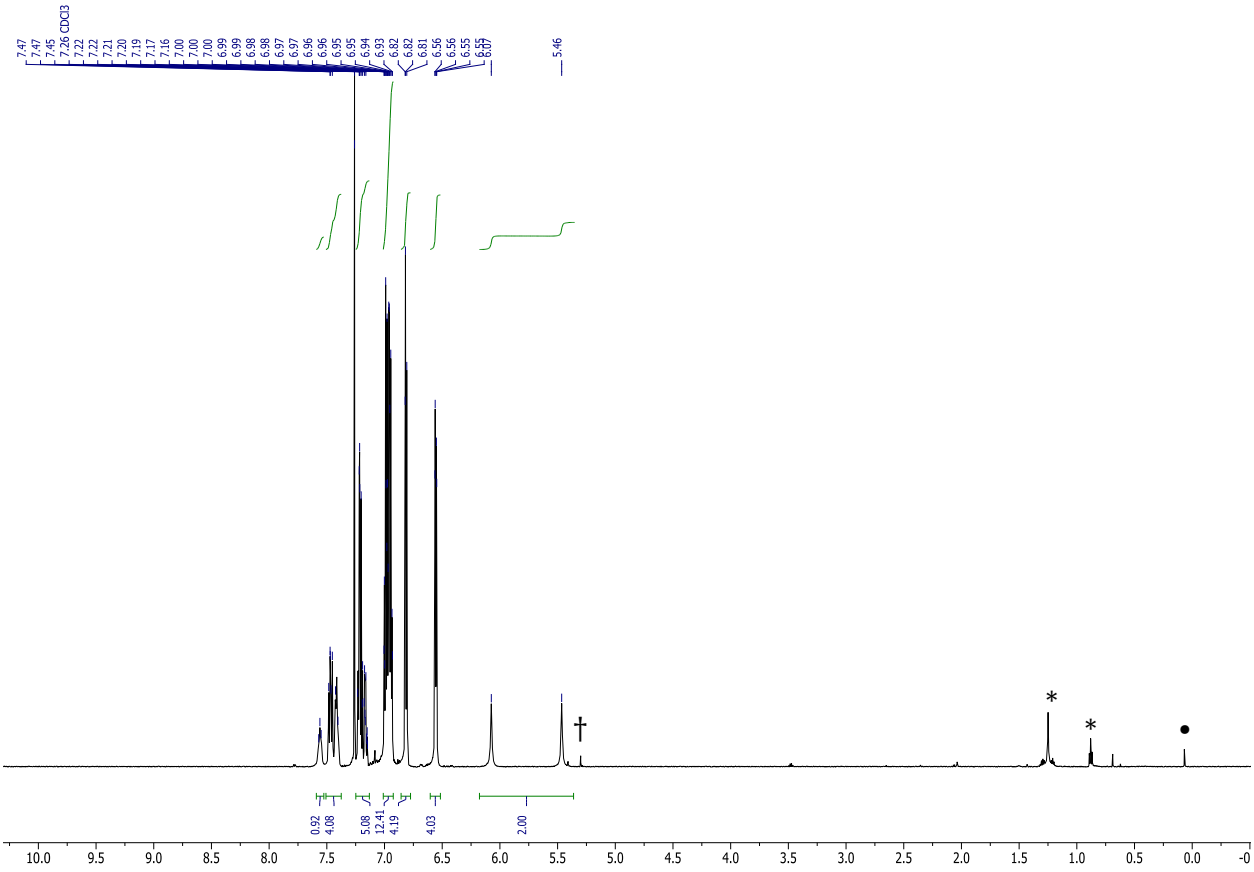


Figure S-24: Expansion of ^{1}H NMR spectrum of **15** in $CDCl_3$.

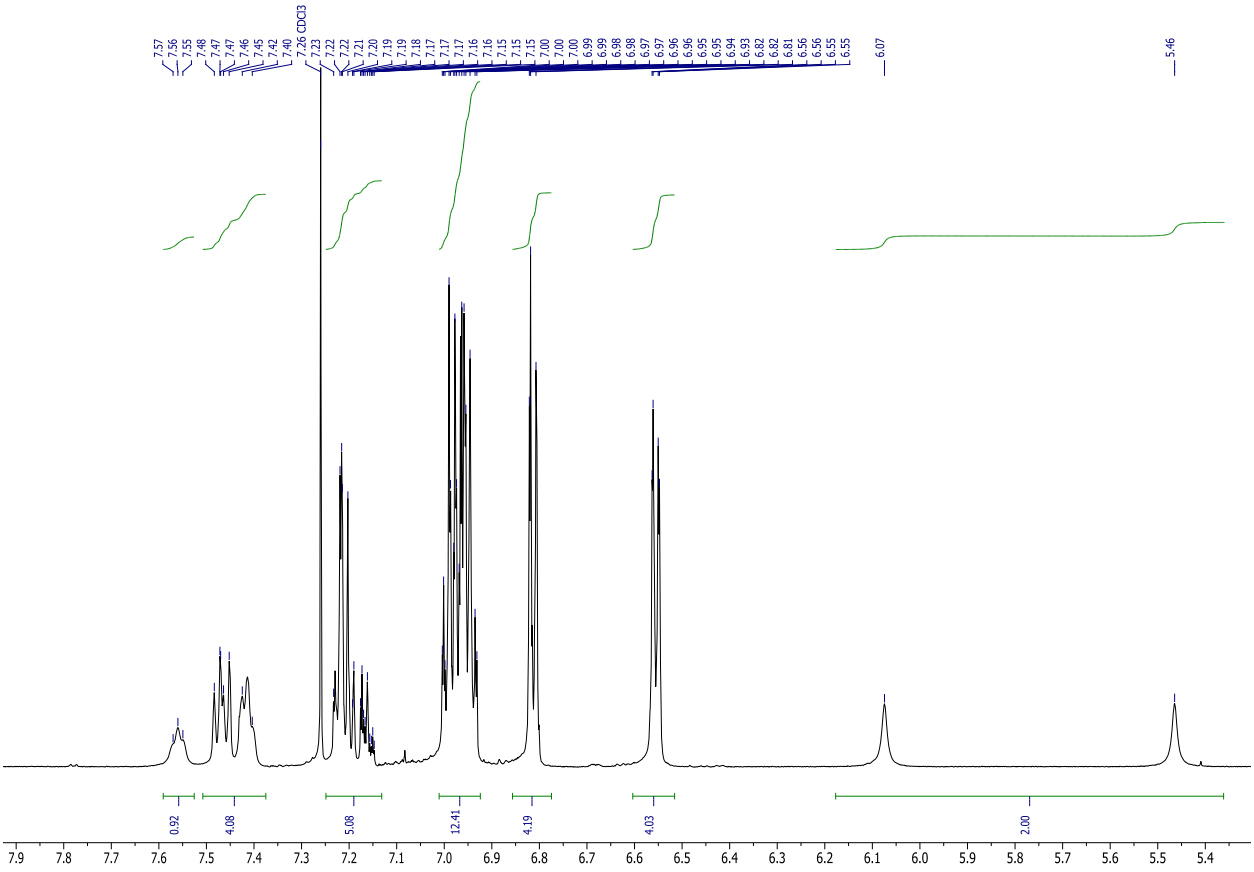


Figure S-25: $^{11}B\{^{1}H\}$ NMR spectrum of **15** in $CDCl_3$.

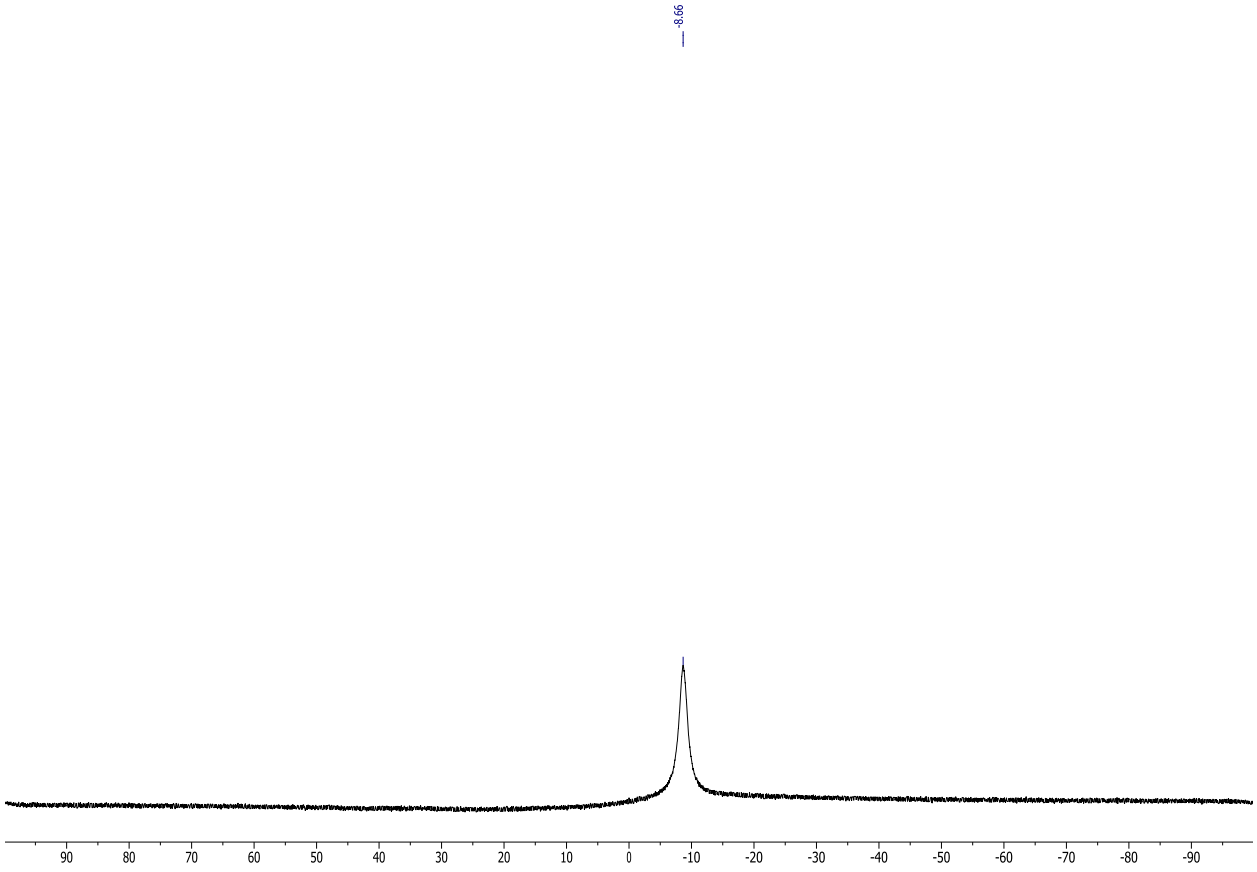


Figure S-26: $^{31}P\{^{1}H\}$ NMR spectrum of **15** in $CDCl_3$.

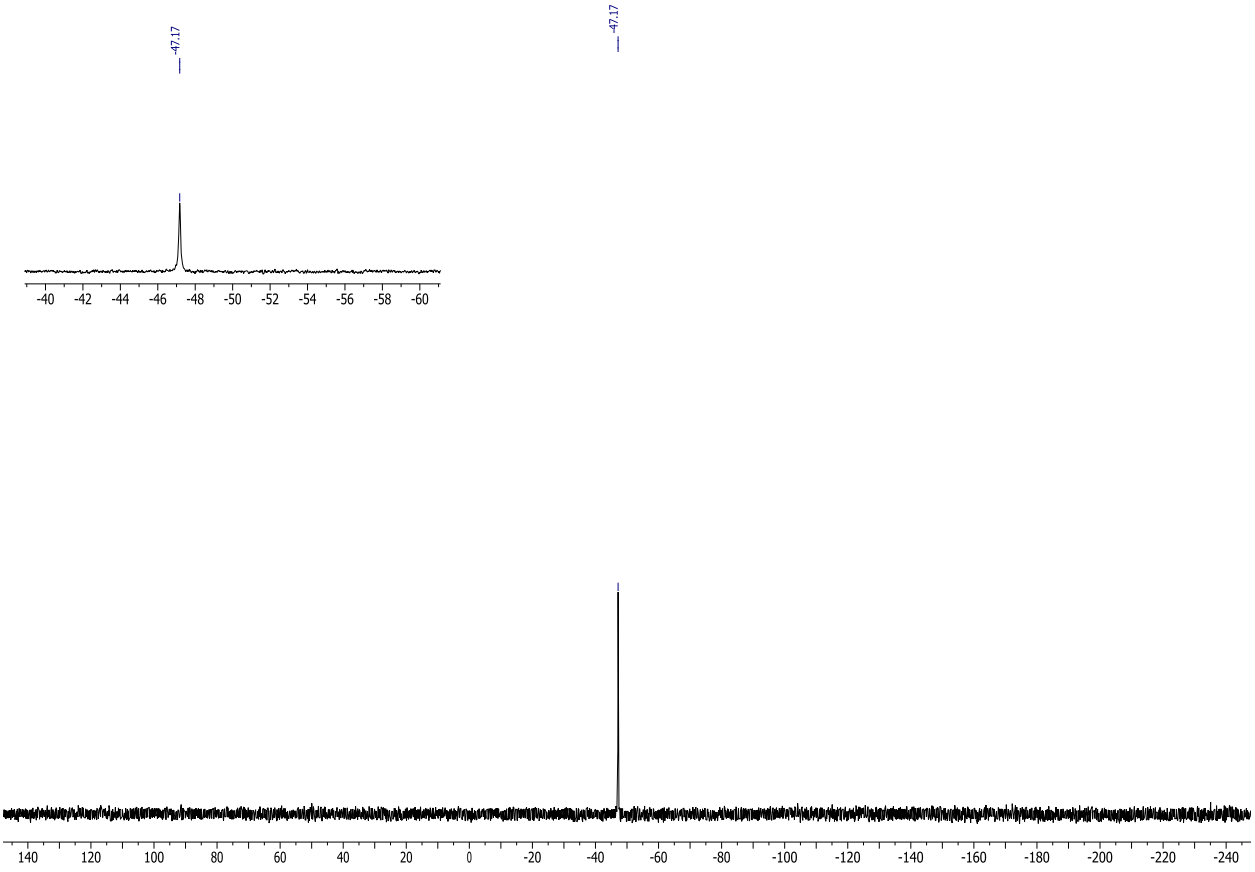


Figure S-27: ^{31}P NMR spectrum of **15** in $CDCl_3$.

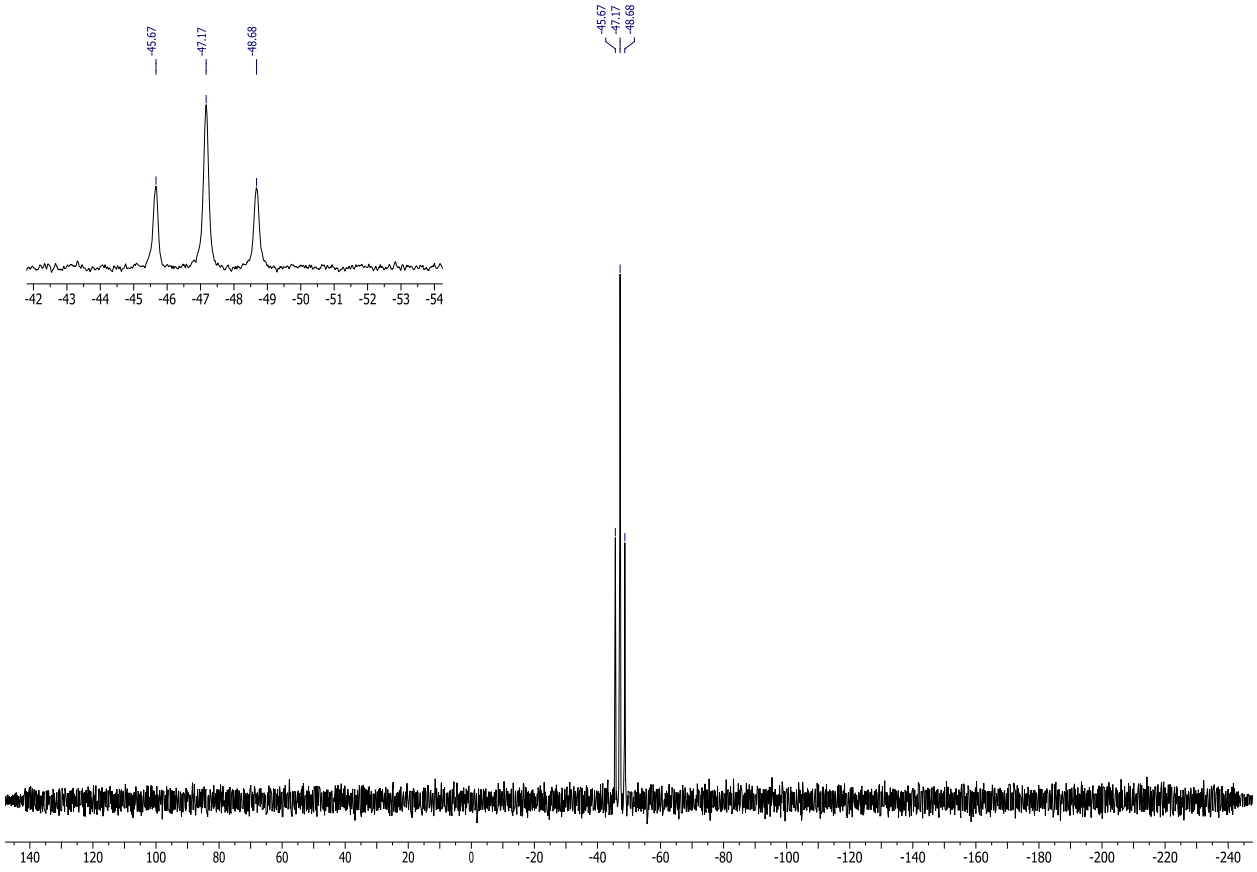


Figure S-28: $^{13}C\{^{1}H\}$ NMR spectrum of **15** in $CDCl_3$.

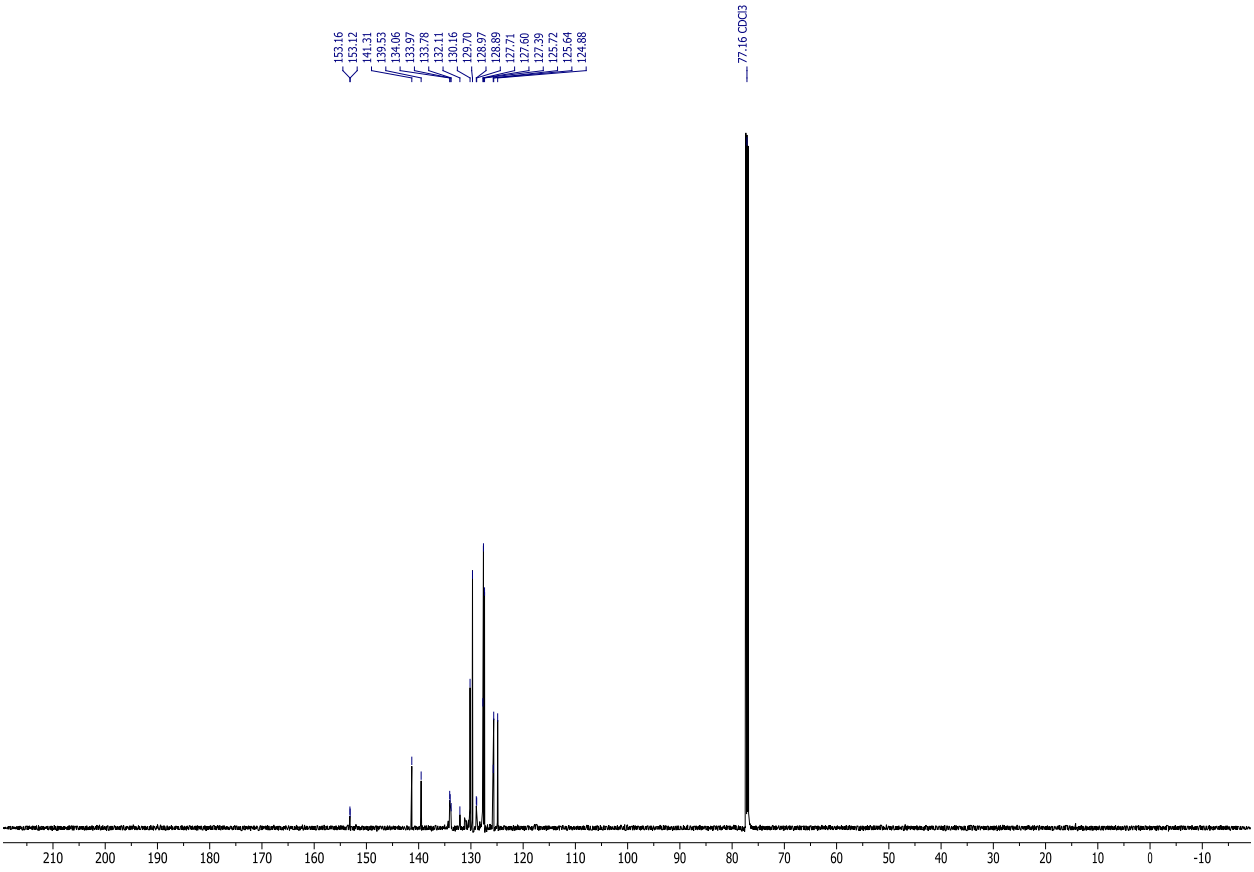


Figure S-29: Expansion of $^{13}C\{^{1}H\}$ NMR spectrum of **15** in $CDCl_3$.

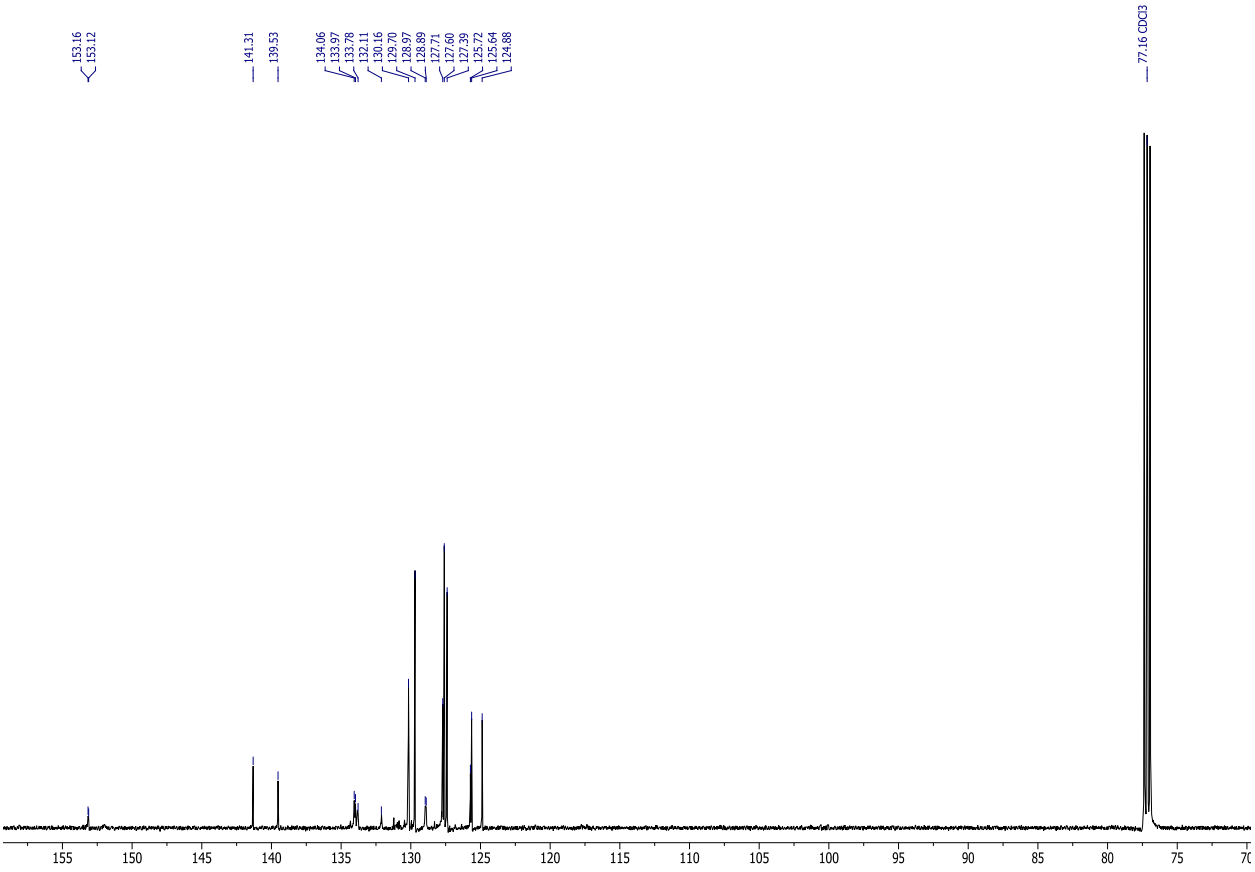
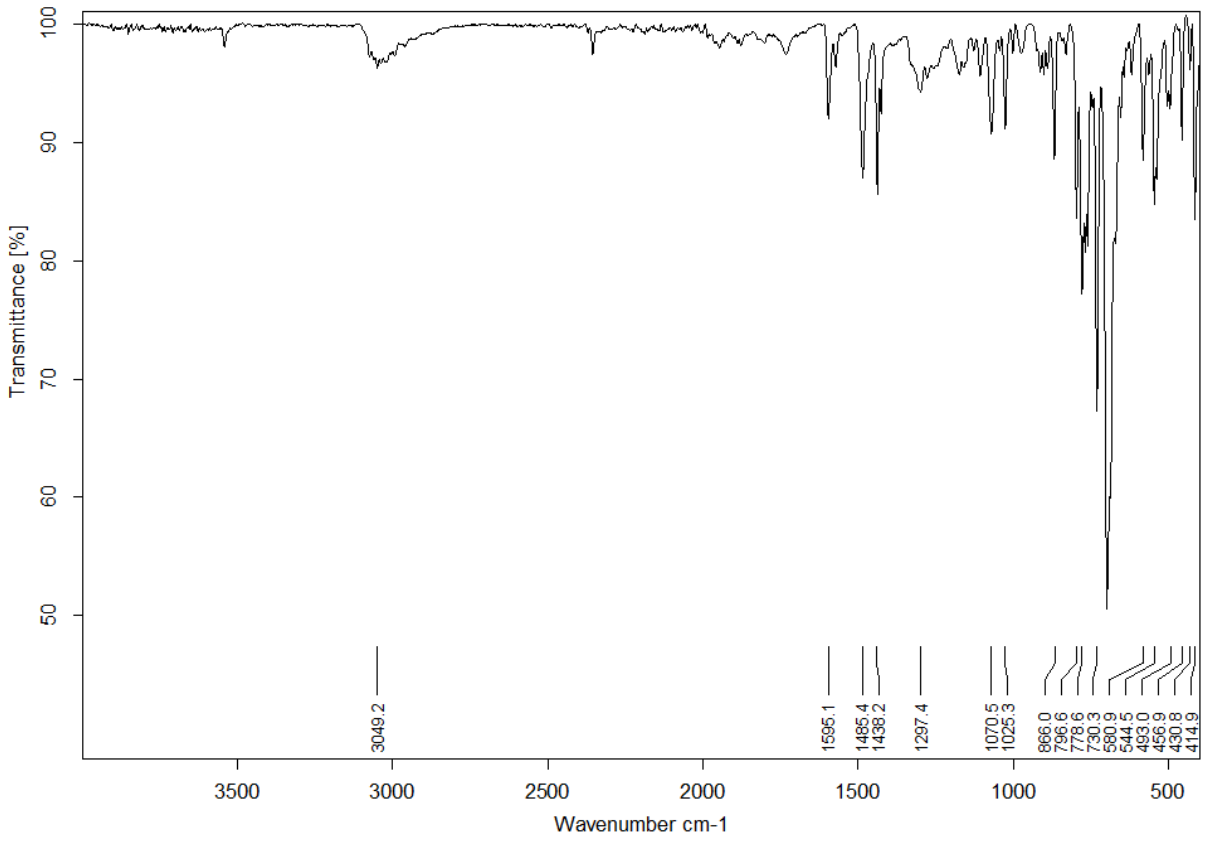


Figure S-30: FT-IR spectrum of **15**.



X-Ray Crystallography details: Crystals were selected under paratone oil, mounted on micromounts then immediately placed in a cold stream of N_2. Structures were solved and refined using SHELXTL[1]. For compounds **12** and **15**, the *n*-pentane and *n*-hexane solvates were found to be disordered to an extent that could not be modeled and the contribution of the solvate was removed from the reflection data using the squeeze function in the PLATON software suite.[2] For compound **14**, the toluene solvent molecule in the unit cell was disordered on an inversion center and was removed from the reflection data using the squeeze function in the PLATON software suite.[2]

Table S-1: Crystallographic data for **11**-**15**.

Compound	**11**	**12**	**13**	**14**	**15**
CCDC	1443358	1443359	1443360	1443361	1443362
Empirical formula	$C_{34}H_{27}BO$	$C_{68}H_{52}B_2O$	$C_{44}H_{33}BS$	$C_{40}H_{32}BN$	$C_{40}H_{32}BP$
FW (g/mol)	462.36	906.71	604.57	537.47	554.43
Crystal system	Monoclinic	Monoclinic	Triclinic	Triclinic	Monoclinic
Space group	*P2₁/n*	*C2/c*	*P-1*	*P-1*	*C2/c*
a (Å)	16.1884(9)	47.9860(16)	8.5301(6)	10.1357(6)	14.7877(6)
b (Å)	9.1325(6)	10.1805(3)	9.7269(7)	12.1343(7)	12.3571(6)
c (Å)	18.4471(13)	22.1076(7)	19.5345(15)	14.8636(9)	35.9892(16)
α (deg)	90	90	87.469(2)	70.2320(17)	90
β (deg)	108.626(2)	91.302(2)	86.921(2)	73.1203(19)	95.394(3)
γ (deg)	90	90	82.647(2)	85.9647(18)	90
V (Å^3)	2584.4(3)	10797.2(6)	1604.0(2)	1645.44(17)	6547.3(5)
Z	4	8	2	2	8
D_c (mg m^{-3})	1.188	1.230	1.252	1.085	1.125
radiation, λ (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
temp (K)	150(2)	150(2)	150(2)	150(2)	150(2)
$R1[I>2\sigma I]$[a]	0.0529	0.0876	0.0562	0.0488	0.0717
$wR2(F^2)$[a]	0.1502	0.1365	0.1539	0.1279	0.1297
GOF (*S*)[a]	1.085	1.047	1.055	1.088	1.124

[a] $R1(F[\mathrm{I} > 2(\mathrm{I})]) = \sum\|\|F_o| - |F_c\|\| / \sum |F_o|$; $wR2(F^2\ [\text{all data}]) = [w(F_o^2 - F_c^2)^2]^{1/2}$; $S(\text{all data}) = [w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = no. of data; p = no. of parameters varied; $w = 1/[^2(F_o^2) + (aP)^2 + bP]$ where $P = (F_o^2 + 2F_c^2)/3$ and a and b are constants suggested by the refinement program.

References:

1. Sheldrick, G. M. *Acta Crystallogr.* **2008**, *A64*, 112.

2. Spek, A. L. *Acta Crystallogr.* **2009**, *D65*, 148.

Cartesian Coordinates of M06-2X / 6-31+G(d) optimised geometries

Reactants

2,3,4,5-tetramethyl-1-phenylborane

E_{SCF} = -568.311763727 Hartree
Singlet, neutral

6	3.618646	1.497053	-0.160491
6	2.316844	0.760468	-0.063760
6	2.316835	-0.760458	0.063713
6	1.064900	-1.262522	0.081890
5	0.106853	0.000033	0.000157
6	1.064922	1.262574	-0.081610
6	0.696584	2.711556	-0.239272
1	1.534200	3.322980	-0.589491
1	-0.122103	2.831485	-0.958302
1	0.351515	3.147895	0.707687
6	-1.449007	0.000019	0.000076
6	-2.180700	-1.110302	-0.461240
6	-3.572946	-1.109097	-0.477689
6	-4.271000	-0.000047	-0.000173
6	-3.573081	1.109039	0.477457
6	-2.180833	1.110312	0.461248
1	-1.649250	1.984865	0.826872
1	-4.114994	1.973220	0.851729
1	-5.357700	-0.000073	-0.000268
1	-4.114752	-1.973298	-0.852069
1	-1.649010	-1.984823	-0.826788
6	0.696561	-2.711492	0.239711
1	0.351834	-3.148049	-0.707275
1	1.534083	-3.322807	0.590349
1	-0.122356	-2.831306	0.958494
6	3.618626	-1.497107	0.160099
1	4.255380	-1.279208	-0.706217
1	4.181442	-1.188278	1.050184
1	3.476222	-2.578512	0.207183
1	4.181163	1.188255	-1.050777
1	3.476294	2.578470	-0.207459
1	4.255657	1.279053	0.705609

H_2O

E_{SCF} = -76.3837661933 Hartree
Singlet, neutral

8	0.000000	0.116389	0.000000
1	0.770604	-0.465524	0.000000
1	-0.770604	-0.465586	0.000000

thiophenol (PhSH))

E_{SCF} = -630.296445793 Hartree
Singlet, neutral

16	2.282897	-0.082928	-0.004779
6	0.509059	-0.000242	0.001300
6	-0.197786	-1.207061	0.002887
6	-0.192317	1.208408	-0.002003
6	-1.589731	-1.200157	0.000920
6	-1.585463	1.205879	-0.000996
1	0.344887	2.153096	-0.005752
6	-2.291334	0.004640	-0.000416
1	-2.118639	2.152200	-0.002200
1	-3.376766	0.007024	-0.000585
1	0.341627	-2.150493	0.007529
1	-2.126949	-2.144076	0.002144
1	2.494917	1.240294	0.065183

aniline (NH_2Ph)

E_{SCF} = -630.296445793 Hartree
Singlet, neutral

6	-1.169737	1.200785	0.003859
6	0.221724	1.205853	-0.005845
6	0.935284	0.000177	-0.008908
6	0.221618	-1.205811	-0.005711
6	-1.169516	-1.200944	0.003493
6	-1.878419	0.000047	0.008990
1	-1.702940	2.147407	0.007372
1	0.764366	2.148303	-0.017977
1	0.764869	-2.147929	-0.016868
1	-1.703169	-2.147315	0.006603
1	-2.963562	-0.000340	0.016804
7	2.332117	-0.000105	-0.076976
1	2.775217	0.835831	0.283241
1	2.774674	-0.835867	0.284388

phenylphosphine (PH_2Ph)

E_{SCF} = -574.046105321 Hartree
Singlet, neutral

6	1.603028	1.216497	-0.000002
6	0.211259	1.200131	0.000004
6	-0.489442	-0.013543	0.000008
6	0.236904	-1.207998	0.000009
6	1.633143	-1.195069	-0.000001
6	2.317268	0.016775	-0.000007
1	2.132277	2.165136	-0.000005
1	-0.336946	2.139189	0.000005
1	-0.292995	-2.157434	0.000019
1	2.182122	-2.132233	-0.000002
1	3.403303	0.030366	-0.000013
15	-2.334902	-0.119903	0.000012
1	-2.568604	0.826527	1.029332
1	-2.568593	0.826241	-1.029573

H_2O reaction

Intermediate 1 (adduct)

E_{SCF} = -644.711587639 Hartree
Singlet, neutral

5	0.123006	0.003940	0.502062
8	0.002850	0.142304	2.222232
1	-0.796269	0.635972	2.477755
1	0.781089	0.647518	2.517137
6	0.986635	1.280213	0.029611
6	2.178712	0.802632	-0.389626
6	3.313516	1.558792	-1.021723
1	3.483664	1.219139	-2.051508
1	3.125199	2.634508	-1.053116
1	4.252753	1.396790	-0.478531
6	2.288295	-0.691261	-0.192979
6	3.563153	-1.404536	-0.546958
1	3.827004	-1.242587	-1.599467
1	4.407674	-1.036192	0.049823
1	3.483982	-2.482411	-0.387012
6	1.154254	-1.212272	0.320306
6	0.920997	-2.638356	0.727562
1	1.832197	-3.245753	0.721889
1	0.497963	-2.681726	1.740059
1	0.190469	-3.134494	0.075294
6	0.504243	2.699958	-0.059286
1	1.260687	3.394905	-0.438097
1	-0.372589	2.768845	-0.716683
1	0.178447	3.083619	0.920266
6	-1.409136	-0.084486	0.057038
6	-2.342331	0.881599	0.472405
1	-2.016650	1.725404	1.086560
6	-3.682535	0.832675	0.091397
1	-4.376220	1.595613	0.435177
6	-4.124541	-0.188551	-0.747869
1	-5.165776	-0.232126	-1.055067
6	-3.217002	-1.146406	-1.197960
1	-3.550910	-1.940075	-1.861266
6	-1.882933	-1.093044	-0.794273
1	-1.188498	-1.846815	-1.157241

Transition State 1 (TS1, H-migration from Int1)

E_{SCF} = -644.686180576 Hartree
Singlet, neutral

5	-0.085790	-0.303813	0.638245
8	-0.115133	-0.710160	2.199399
1	0.653738	-0.335077	2.660668
1	-0.825532	0.227491	1.884559
6	-1.084968	-1.311987	-0.091965
6	-2.206289	-0.647475	-0.453547
6	-3.427615	-1.182097	-1.148375
1	-3.648803	-0.614198	-2.060352
1	-3.298467	-2.228392	-1.434312
1	-4.315631	-1.117475	-0.506713
6	-2.130626	0.777782	-0.046524
6	-3.114857	1.772406	-0.584953
1	-2.992305	1.878500	-1.670999
1	-4.143169	1.431406	-0.417275
1	-2.993221	2.756896	-0.127929
6	-1.057407	1.079036	0.745027
6	-0.618508	2.486350	1.080740
1	-1.389948	3.045401	1.624419
1	0.280530	2.475188	1.707563
1	-0.364909	3.064540	0.182784
6	-0.805164	-2.774645	-0.216967
1	-1.625067	-3.348205	-0.660109
1	0.097791	-2.941437	-0.817847
1	-0.595854	-3.190364	0.778325
6	1.387264	-0.060164	0.096320
6	2.470936	-0.768919	0.633596
1	2.300147	-1.483329	1.439041
6	3.768048	-0.599269	0.145930
1	4.589913	-1.161567	0.581669
6	4.005826	0.286907	-0.901941
1	5.013084	0.424211	-1.285208
6	2.940072	0.995521	-1.458836
1	3.117547	1.687081	-2.278351
6	1.650605	0.821725	-0.961979
1	0.826262	1.378646	-1.405496

Product 1 (Prod1, ring-open product)

E_{SCF} = -644.768236585 Hartree
Singlet, neutral

6	0.061727	2.337356	2.050295
6	-0.814997	1.287987	1.436032
6	-1.381378	1.285143	0.217057
6	-2.099324	0.076970	-0.270466
6	-1.554997	-1.154378	-0.141363
6	-2.304917	-2.400697	-0.593332
1	-3.250723	-2.536182	-0.053208
1	-2.547891	-2.357317	-1.661421
1	-1.708715	-3.306384	-0.441285
5	-0.125682	-1.384312	0.482021
8	0.025565	-2.265467	1.525665
1	-0.814880	-2.614844	1.851923
6	1.208184	-0.758781	-0.065365
6	2.395062	-0.873745	0.674123
1	2.375042	-1.409599	1.620030
6	3.586766	-0.311923	0.218622
6	3.613867	0.368775	-0.998338
1	4.541706	0.805554	-1.357767
6	2.447766	0.483064	-1.756415
1	2.467434	1.005557	-2.709069
6	1.260467	-0.075291	-1.288809
1	0.352398	0.016700	-1.881708
1	4.494412	-0.406085	0.808659
6	-3.437037	0.324524	-0.930355

1	-4.036852	-0.585579	-0.995534
1	-4.013587	1.075116	-0.378424
1	-3.304566	0.706057	-1.951501
6	-1.330030	2.446125	-0.746280
1	-2.335882	2.836596	-0.941478
1	-0.718187	3.269904	-0.377133
1	-0.916597	2.126961	-1.711126
1	-0.980129	0.410202	2.062083
1	-0.281947	2.594512	3.058167
1	1.083701	1.946988	2.147072
1	0.112197	3.256360	1.463869

Product 2 (Prod2, ring-closed product)

E_{SCF} = -644.787635586 Hartree
Singlet, neutral

6	-0.077757	0.294173	0.792333
6	-0.980014	-0.935185	0.683744
6	-0.656497	-2.129637	1.532960
1	-0.807698	-1.903496	2.595973
1	-1.263597	-3.004328	1.289102
1	0.399883	-2.401698	1.412123
6	-1.984541	-0.809263	-0.204631
6	-3.027949	-1.835220	-0.541730
1	-4.025057	-1.496792	-0.233391
1	-3.070348	-1.994085	-1.627361
1	-2.844447	-2.800295	-0.064397
6	-2.003208	0.523818	-0.942577
1	-1.712574	0.351709	-1.995059
6	-3.368701	1.229120	-0.942661
1	-3.721176	1.402910	0.080981
1	-3.317666	2.201613	-1.448019
1	-4.133114	0.641130	-1.462562
5	-0.856091	1.299563	-0.165568
8	-0.582259	2.627670	-0.187361
6	1.299039	0.038808	0.182079
6	2.465159	0.611659	0.705050
1	2.414610	1.230825	1.594726
6	3.704797	0.401202	0.101446
1	4.592845	0.855399	0.532505
6	3.809092	-0.385179	-1.043106
1	4.775105	-0.549975	-1.511228
6	2.657383	-0.960029	-1.578480
1	2.720443	-1.578900	-2.469439
6	1.421239	-0.749425	-0.972888
1	0.532362	-1.214502	-1.393961
6	-0.004313	0.824982	2.232332
1	-1.010633	0.877696	2.662718
1	0.605238	0.176846	2.874602
1	0.418275	1.834137	2.264126
1	-1.136295	3.133683	-0.797937

Product 3 (Prod3, bis-borole product)

E_{SCF} = -1213.12019435 Hartree
Singlet, neutral

6	2.853151	1.883162	-1.964085
6	2.118366	0.592382	-1.755168
1	1.065324	0.701985	-1.491745
6	2.597460	-0.658133	-1.858787
6	1.721986	-1.813084	-1.514670
6	1.006862	-1.795348	-0.368166
5	1.143357	-0.626150	0.683844
8	0.000000	0.000000	1.091821
5	-1.143357	0.626150	0.683844
6	-1.006862	1.795348	-0.368166
6	-1.721986	1.813084	-1.514670
6	-2.597460	0.658133	-1.858787
6	-2.118366	-0.592382	-1.755168
1	-1.065324	-0.701985	-1.491745
6	-2.853151	-1.883162	-1.964085
1	-3.799545	-1.759585	-2.494013
1	-2.236363	-2.588287	-2.531407
1	-3.071643	-2.353841	-0.996432
6	-3.993981	0.992070	-2.323705
1	-3.974614	1.480072	-3.305312
1	-4.628012	0.108273	-2.400945
1	-4.476426	1.688656	-1.628222
6	-1.723613	2.935968	-2.525732
1	-2.697532	3.440046	-2.538827
1	-0.967414	3.693720	-2.319832
1	-1.553015	2.545646	-3.535501
6	0.000000	2.853425	0.030919
1	0.224587	3.576199	-0.756560
1	-0.346805	3.414322	0.908229
1	0.944873	2.376996	0.322855
6	-2.469319	0.262868	1.444930
6	-3.645140	1.006921	1.274562
1	-3.631008	1.865716	0.607391
6	-4.816572	0.670852	1.944623
1	-5.716579	1.261567	1.800739
6	-4.832606	-0.426330	2.804961
1	-5.746022	-0.693216	3.328699
6	-3.674063	-1.175152	2.997827
1	-3.682432	-2.025647	3.673182
6	-2.505195	-0.826645	2.326331
1	-1.597479	-1.403432	2.488158
6	2.469319	-0.262868	1.444930
6	2.505195	0.826645	2.326331
1	1.597479	1.403432	2.488158
6	3.674063	1.175152	2.997827
1	3.682432	2.025647	3.673182
6	4.832606	0.426330	2.804961
1	5.746022	0.693216	3.328699
6	4.816572	-0.670852	1.944623
1	5.716579	-1.261567	1.800739
6	3.645140	-1.006921	1.274562
1	3.631008	-1.865716	0.607391
6	0.000000	-2.853425	0.030919

1	-0.944873	-2.376996	0.322855
1	-0.224587	-3.576199	-0.756560
1	0.346805	-3.414322	0.908229
6	1.723613	-2.935968	-2.525732
1	1.553015	-2.545646	-3.535501
1	2.697532	-3.440046	-2.538827
1	0.967414	-3.693720	-2.319832
6	3.993981	-0.992070	-2.323705
1	4.628012	-0.108273	-2.400945
1	4.476426	-1.688656	-1.628222
1	3.974614	-1.480072	-3.305312
1	2.236363	2.588287	-2.531407
1	3.071643	2.353841	-0.996432
1	3.799545	1.759585	-2.494013

Intermediate 3 (Ph migration)

E_{SCF} = -644.678173148 Hartree
Singlet, neutral

6	-0.122966	-0.242751	0.894435
6	-1.175870	-1.150765	0.265019
6	-1.039257	-2.638388	0.390082
1	-1.088510	-2.969133	1.437850
1	-1.820663	-3.173659	-0.156346
1	-0.070172	-2.982063	-0.000747
6	-2.177869	-0.424755	-0.296539
6	-3.411163	-0.984816	-0.950713
1	-4.314006	-0.634427	-0.434858
1	-3.490958	-0.645983	-1.991206
1	-3.427699	-2.077239	-0.950565
6	-1.979533	1.050269	-0.227813
6	-2.945620	2.005689	-0.871252
1	-3.956197	1.934174	-0.445539
1	-2.632172	3.050265	-0.742797
1	-3.047858	1.835714	-1.952438
5	-0.761515	1.159342	0.510344
8	0.151881	2.397780	0.755254
6	1.222195	-0.260228	0.194279
6	2.396859	0.162655	0.841511
1	2.386629	0.359464	1.911135
6	3.609438	0.278652	0.147855
1	4.502904	0.591954	0.681572
6	3.673997	-0.023098	-1.206515
1	4.613469	0.057961	-1.744993
6	2.512953	-0.443082	-1.865199
1	2.549428	-0.683922	-2.924293
6	1.309714	-0.552745	-1.179777
1	0.404776	-0.863251	-1.697016
6	-0.035548	-0.494052	2.410340
1	-1.048060	-0.515306	2.825367
1	0.449706	-1.453776	2.631219
1	0.517001	0.287679	2.944430
1	-0.044537	3.107406	0.118521
1	1.085477	2.099684	0.622682

SHPh reaction

Intermediate 1 (adduct)

E_{SCF} = -1198.62846574 Hartree
Singlet, neutral

5	0.909672	0.196451	0.295373
6	0.204529	1.634782	0.277930
6	-0.861127	1.545591	1.105885
6	-1.873273	2.604244	1.438000
1	-1.884737	2.821408	2.513425
1	-1.678295	3.540468	0.909468
1	-2.885602	2.270783	1.171708
6	-0.987598	0.173169	1.707240
6	-2.163644	-0.167051	2.576738
1	-2.231064	0.503912	3.442014
1	-3.103508	-0.062391	2.016769
1	-2.108391	-1.191791	2.952933
6	0.012244	-0.646096	1.312919
6	0.143509	-2.101532	1.669679
1	-0.825570	-2.584990	1.845194
1	0.655076	-2.661652	0.874206
1	0.745103	-2.251491	2.576594
6	0.643892	2.841210	-0.498898
1	0.032891	3.728316	-0.302496
1	1.686150	3.094809	-0.266936
1	0.610851	2.655473	-1.583482
6	2.464325	-0.033683	0.052752
6	3.149627	0.531517	-1.037675
1	2.598528	1.125244	-1.765902
6	4.519910	0.354214	-1.216132
1	5.019251	0.802282	-2.071151
6	5.251324	-0.393611	-0.292762
1	6.320910	-0.531343	-0.425284
6	4.600133	-0.959754	0.801202
1	5.162222	-1.539814	1.528391
6	3.225103	-0.784847	0.962595
1	2.733177	-1.229772	1.824221
6	-1.677307	-0.646290	-1.333418
6	-2.421753	0.517233	-1.526504
1	-1.938975	1.420247	-1.890673
6	-3.784263	0.515319	-1.230662
1	-4.363549	1.422141	-1.376912
6	-4.398566	-0.640401	-0.752941
1	-5.460223	-0.638365	-0.525350
6	-3.646476	-1.800649	-0.566229
6	-2.283376	-1.805691	-0.847730
1	-1.693883	-2.702409	-0.674463
1	-4.117801	-2.703000	-0.188415
16	0.070790	-0.552082	-1.635845
1	0.343153	-1.863062	-1.499125

TS1 (H-migration from Int1)

E_{SCF} = -1198.60693916 Hartree
Singlet, neutral

5	-1.002452	0.247374	0.321311
6	0.005824	-0.298765	1.395109
6	0.998233	0.619323	1.540499
6	2.257718	0.483971	2.346401
1	2.409126	1.350186	3.001358
1	2.236877	-0.409224	2.974568
1	3.134079	0.412890	1.688013
6	0.762470	1.809704	0.702406
6	1.661635	3.001621	0.817934
1	1.563013	3.464271	1.808189
1	2.709394	2.692676	0.716350
1	1.450652	3.759802	0.062033
6	-0.333755	1.676918	-0.123682
6	-0.969188	2.769130	-0.946154
1	-1.049051	2.486316	-2.003346
1	-1.986883	2.971509	-0.592375
1	-0.407593	3.706579	-0.901324
6	-0.006150	-1.677796	1.982568
1	0.996063	-2.044589	2.229150
1	-0.606318	-1.712571	2.901553
1	-0.464965	-2.381311	1.277206
6	-2.517651	-0.082509	0.101274
6	-3.254148	-0.685361	1.132610
1	-2.756231	-0.936497	2.066240
6	-4.613972	-0.960720	0.991045
1	-5.162286	-1.421953	1.807849
6	-5.265911	-0.649478	-0.200134
1	-6.323642	-0.867999	-0.317408
6	-4.553097	-0.057515	-1.243861
1	-5.054261	0.182677	-2.177415
6	-3.199495	0.226751	-1.088089
1	-2.658799	0.684467	-1.914513
6	1.761899	-0.899705	-1.146015
6	2.346978	-1.990637	-0.487748
1	1.730325	-2.847395	-0.230221
6	3.701380	-1.975196	-0.169290
1	4.144402	-2.829514	0.334845
6	4.489431	-0.868232	-0.492972
1	5.546362	-0.859319	-0.243165
6	3.913846	0.220543	-1.144438
6	2.557849	0.205993	-1.473126
1	2.112589	1.047355	-1.998232
1	4.521544	1.081471	-1.409850
16	0.034578	-0.912635	-1.541993
1	-0.088770	0.627216	-0.980186

Product 1 (Prod1, ring opened product)

E_{SCF} = -1198.66272915 Hartree
Singlet, neutral

6	2.226496	1.260946	2.661616
6	1.152376	1.373354	1.623141
6	1.255033	2.025426	0.453130
6	0.195038	1.921115	-0.577426
6	-0.314412	0.722210	-0.951317
6	-1.408541	0.665886	-2.003082
1	-2.360714	1.063047	-1.625091
1	-1.131504	1.259347	-2.882830
1	-1.597147	-0.357662	-2.338634
5	0.218826	-0.613607	-0.339821
16	-0.924210	-1.872147	0.320969
6	-2.524804	-1.075854	0.333100
6	-2.758164	0.078811	1.084227
6	-4.013353	0.682625	1.062879
6	-5.047185	0.129518	0.307267
1	-6.025100	0.601455	0.293132
6	-4.821233	-1.035819	-0.423221
6	-3.563897	-1.637715	-0.411681
1	-3.379621	-2.536913	-0.993132
1	-5.621938	-1.475756	-1.010627
1	-4.183510	1.585409	1.642503
1	-1.956008	0.512208	1.673832
6	1.729893	-1.044289	-0.361602
6	2.256834	-2.008595	0.514684
1	1.607226	-2.474003	1.253188
6	3.601821	-2.369504	0.473736
1	3.985434	-3.111185	1.168878
6	4.454164	-1.779300	-0.459161
1	5.502691	-2.061670	-0.495648
6	3.953899	-0.825378	-1.345030
1	4.611715	-0.363711	-2.076528
6	2.610021	-0.462426	-1.290183
1	2.230614	0.291330	-1.977094
6	-0.292804	3.213986	-1.196670
1	0.081775	4.086239	-0.654495
1	0.015633	3.308145	-2.246207
1	-1.388018	3.253598	-1.181720
6	2.489674	2.819653	0.080974
1	2.335813	3.389720	-0.839344
1	2.790802	3.520734	0.866031
1	3.329321	2.134664	-0.096144
1	0.229966	0.832175	1.831599
1	3.018547	2.001507	2.524776
1	1.821036	1.369816	3.672648
1	2.691088	0.265996	2.602222

Product 2 (Prod2, ring closed product)

E_{SCF} = -1198.68090192 Hartree
Singlet, neutral

6	-1.482594	0.481043	0.811685
6	-1.775258	1.828011	0.146266
6	-3.159263	2.396337	0.269363
1	-3.360034	2.715680	1.299848
1	-3.320458	3.259368	-0.380758
1	-3.907368	1.634222	0.018015
6	-0.723792	2.365479	-0.496548
6	-0.692693	3.670870	-1.239193
1	-0.112766	4.423418	-0.690774
1	-0.205178	3.543791	-2.214215
1	-1.690128	4.082646	-1.409736
6	0.549937	1.531493	-0.426858
1	0.840850	1.216376	-1.443889
6	1.737986	2.309287	0.172588
1	1.515654	2.626443	1.198587
1	2.645995	1.699869	0.192795
1	1.953551	3.208711	-0.414952
5	0.062636	0.301847	0.444941
16	0.974111	-1.115931	1.057114
6	2.597548	-0.943872	0.325698
6	2.764114	-1.005602	-1.059537
6	4.034688	-0.862274	-1.613082
1	4.158090	-0.902324	-2.691473
6	5.143667	-0.676710	-0.787947
6	4.978591	-0.641808	0.595811
6	3.708428	-0.775461	1.154299
1	3.573047	-0.733361	2.231300
1	5.838635	-0.503463	1.244489
1	6.133004	-0.566733	-1.221706
1	1.899524	-1.165048	-1.698300
6	-2.272641	-0.643341	0.143571
6	-2.898512	-1.663393	0.867904
1	-2.867709	-1.660408	1.952792
6	-3.571363	-2.698771	0.217200
1	-4.051228	-3.476601	0.804799
6	-3.631206	-2.737998	-1.172822
1	-4.155365	-3.543897	-1.677970
6	-3.011880	-1.727974	-1.909060
1	-3.051936	-1.741989	-2.994829
6	-2.343266	-0.696105	-1.257389
1	-1.875325	0.094487	-1.841165
6	-1.712578	0.555408	2.331062
1	-1.177736	1.416508	2.746412
1	-2.777293	0.669526	2.570174
1	-1.344246	-0.339275	2.843957

Intermediate 3 (Ph migration from Int1)

E_{SCF} = -1198.5929058 Hartree
Singlet, neutral

5	0.035882	0.618515	0.470521
6	1.001063	0.163572	-0.717013
6	1.780837	1.469496	-0.897372
6	2.851158	1.541570	-1.942803
1	3.396685	2.488476	-1.917453
1	3.579715	0.730255	-1.807804
1	2.435616	1.427261	-2.953987
6	1.354602	2.441930	-0.052307
6	1.877946	3.850103	0.024058
1	2.684220	4.035269	-0.689430
1	1.079784	4.575596	-0.177774
1	2.260271	4.072257	1.028208
6	0.259577	1.990923	0.844431
6	-0.339167	2.914361	1.864604
1	0.404558	3.278664	2.586580
1	-0.787589	3.805237	1.402743
1	-1.135552	2.426561	2.442588
6	0.221681	-0.151588	-2.006835
1	0.892621	-0.401637	-2.839552
1	-0.472474	-0.991820	-1.878343
1	-0.368906	0.724000	-2.297739
6	1.915747	-0.970331	-0.276741
6	2.814228	-0.750639	0.781964
1	2.841379	0.236340	1.240579
6	3.653294	-1.758755	1.238099
1	4.340610	-1.558717	2.055924
6	3.616683	-3.027183	0.649766
1	4.272748	-3.816825	1.004578
6	2.733544	-3.261705	-0.396807
1	2.695507	-4.239772	-0.869345
6	1.892811	-2.241790	-0.856690
1	1.220774	-2.451886	-1.683417
6	-2.733367	-0.533795	0.449333
6	-3.077303	0.583083	-0.305285
1	-2.382335	1.419014	-0.371431
6	-4.301821	0.592023	-0.969731
1	-4.585703	1.457894	-1.560146
6	-5.155744	-0.508108	-0.883769
1	-6.106037	-0.497676	-1.409047
6	-4.790904	-1.624218	-0.132492
6	-3.569517	-1.643336	0.540108
1	-3.269692	-2.509914	1.123064
1	-5.452052	-2.483276	-0.072414
16	-1.141413	-0.590428	1.324214
1	-1.493037	0.175292	2.376476

Intermediate 2 (H migration from Int1)

E_{SCF} = -1198.65663263 Hartree
Singlet, neutral

5	-0.899049	0.195063	-0.126033
6	-0.207552	1.295856	0.748594
6	0.937907	1.832600	-0.035432
6	1.817885	2.904361	0.540202
1	2.690959	3.104235	-0.085081
1	1.266317	3.845868	0.656696
1	2.176443	2.629043	1.540180
6	1.060384	1.199759	-1.223165
6	2.179167	1.350058	-2.208286
1	2.860240	2.168695	-1.964335
1	2.764958	0.420241	-2.234727
1	1.795750	1.516241	-3.221499
6	-0.053319	0.202145	-1.497453
6	-0.958697	0.681604	-2.650652
1	-1.762298	-0.039479	-2.831325
1	-1.426441	1.642510	-2.403764
1	-0.400035	0.810472	-3.584941
6	-0.819886	2.123624	1.850550
1	-0.086563	2.444213	2.598588
1	-1.258018	3.023084	1.398676
1	-1.624750	1.582442	2.356859
6	-2.405587	-0.268273	-0.005727
6	-3.432423	0.687359	0.025464
1	-3.175500	1.745852	0.025017
6	-4.777315	0.315784	0.049924
1	-5.551537	1.078138	0.072570
6	-5.125723	-1.033310	0.050124
1	-6.171059	-1.328449	0.073825
6	-4.122796	-2.003098	0.021905
1	-4.386342	-3.057463	0.024304
6	-2.783826	-1.619234	-0.008125
1	-2.010358	-2.385862	-0.024009
6	1.807174	-0.975507	0.829707
6	2.976647	-0.304257	1.197773
1	2.921422	0.526350	1.894754
6	4.203078	-0.702881	0.673094
1	5.107368	-0.172469	0.956755
6	4.270947	-1.783803	-0.206570
1	5.228957	-2.095421	-0.612094
6	3.108330	-2.468370	-0.556985
6	1.877096	-2.062210	-0.045533
1	0.964883	-2.582697	-0.325044
1	3.156168	-3.315801	-1.234461
16	0.233091	-0.500169	1.503188
1	0.376286	-0.765604	-1.794250

NH_2Ph reaction

Intermediate 1 (adduct)

E_{SCF} = -855.827803989 Hartree
Singlet, neutral

7	-0.222563	-1.464846	-0.434711
5	0.577013	-0.036937	-0.068754
6	0.180785	1.053973	-1.188183
6	-0.474132	2.055677	-0.563381
6	-1.011412	3.327493	-1.158857
1	-0.548427	4.209999	-0.699627
1	-0.832808	3.382754	-2.235725
1	-2.092745	3.416275	-0.992053
6	-0.631220	1.782200	0.906406
6	-1.331141	2.781406	1.785863
1	-0.838274	3.761050	1.748484
1	-2.367382	2.936051	1.459127
1	-1.357523	2.460797	2.829968
6	-0.077585	0.601071	1.259128
6	0.007302	0.026231	2.643115
1	-0.442623	0.662828	3.412283
1	-0.491103	-0.952197	2.708036
1	1.055558	-0.147761	2.923638
6	0.554484	0.972157	-2.638599
1	0.158868	1.793153	-3.246444
1	1.646410	0.962297	-2.755296
1	0.198917	0.034689	-3.100815
6	2.146079	-0.405215	-0.003557
6	2.748628	-1.455653	-0.713443
1	2.150408	-2.114151	-1.346682
6	4.123624	-1.699114	-0.661763
1	4.550127	-2.524792	-1.225718
6	4.944897	-0.879141	0.106289
1	6.014872	-1.061534	0.151882
6	4.377600	0.181818	0.814697
1	5.009003	0.831698	1.415271
6	3.004579	0.406538	0.758921
1	2.575555	1.238051	1.316177
6	-1.670354	-1.441679	-0.297639
6	-2.434824	-0.748734	-1.231446
1	-1.952664	-0.236549	-2.057890
6	-3.818020	-0.701643	-1.073249
1	-4.418217	-0.159340	-1.797336
6	-4.428779	-1.338789	0.005689
1	-5.506863	-1.294906	0.124904
6	-3.651891	-2.036810	0.927979
6	-2.268583	-2.092877	0.775524
1	-1.659724	-2.636418	1.493890
1	-4.118943	-2.540589	1.768471
1	0.171557	-2.195083	0.164550
1	0.028669	-1.721157	-1.393313

TS 1 (H-migration from Int1)

E_{SCF} = -855.780235608 Hartree

Singlet, neutral

7	-0.722062	-0.650195	1.058617
5	0.472262	0.029648	0.186075
6	-0.083461	0.837818	-1.070537
6	0.114952	2.165772	-0.886686
6	-0.227227	3.289677	-1.825503
1	-0.660452	2.915253	-2.755544
1	-0.947189	3.984817	-1.374662
1	0.661837	3.876403	-2.087283
6	0.753054	2.438422	0.418906
6	1.329597	3.793219	0.709180
1	2.170917	4.002699	0.035435
1	0.585407	4.579132	0.535476
1	1.687491	3.873331	1.737857
6	0.870657	1.345550	1.231735
6	1.723761	1.299215	2.478383
1	1.412166	2.039356	3.225198
1	1.663226	0.312559	2.951536
1	2.783773	1.477511	2.256614
6	-0.698135	0.172429	-2.263937
1	-1.338472	-0.662825	-1.956033
1	-1.297757	0.846499	-2.883925
1	0.093328	-0.258173	-2.892187
6	1.713161	-0.951905	-0.037407
6	1.514835	-2.331708	-0.182944
1	0.506742	-2.739681	-0.107845
6	2.577053	-3.200120	-0.442284
1	2.392705	-4.265622	-0.552180
6	3.871072	-2.699372	-0.562976
1	4.702143	-3.370716	-0.760069
6	4.091418	-1.327380	-0.430224
1	5.097562	-0.927656	-0.526123
6	3.024173	-0.470913	-0.171049
1	3.207617	0.598246	-0.073208
6	-2.079416	-0.775834	0.684150
6	-2.818525	0.354600	0.315290
1	-2.342396	1.330923	0.334888
6	-4.147939	0.222335	-0.075350
1	-4.706750	1.107209	-0.366681
6	-4.768228	-1.026913	-0.078465
1	-5.807338	-1.123290	-0.377213
6	-4.041416	-2.148929	0.316076
6	-2.705771	-2.026954	0.691310
1	-2.136857	-2.908120	0.980489
1	-4.510875	-3.128476	0.324234
1	-0.209709	0.522221	1.463491
1	-0.395684	-1.432541	1.621028

Product 1 (Prod1, ring opened product)

E_{SCF} = -855.857441688 Hartree

Singlet, neutral

6	1.829924	0.747178	2.998271
6	1.056163	1.183218	1.790160
6	1.507059	1.840177	0.707105
6	0.604859	2.073260	-0.452316
6	-0.145818	1.068408	-0.957787
6	-1.099660	1.302713	-2.119790
1	-1.849328	2.071633	-1.896604
1	-0.555992	1.626325	-3.016351
1	-1.645310	0.390134	-2.377618
5	0.003142	-0.411064	-0.440435
7	-1.124884	-1.207425	-0.099068
1	-0.966336	-2.206045	-0.009824
6	-2.481340	-0.862171	0.063196
6	-2.876935	0.429733	0.431295
6	-4.228188	0.730626	0.580836
6	-5.204526	-0.245390	0.387312
1	-6.255653	-0.004550	0.511271
6	-4.811882	-1.537248	0.040281
6	-3.464460	-1.842615	-0.123188
1	-3.164444	-2.848907	-0.407792
1	-5.557139	-2.313025	-0.110409
1	-4.516846	1.738625	0.865361
1	-2.125248	1.193148	0.605594
6	1.402325	-1.147045	-0.435128
6	1.685432	-2.194646	0.456160
1	0.936789	-2.494393	1.189087
6	2.921205	-2.839445	0.457167
1	3.117991	-3.637458	1.168106
6	3.906492	-2.454688	-0.451662
1	4.870229	-2.956221	-0.457101
6	3.648870	-1.419711	-1.350072
1	4.411989	-1.115434	-2.061543
6	2.414217	-0.773277	-1.333034
1	2.227200	0.042665	-2.028752
6	0.609685	3.471220	-1.029043
1	0.660516	4.225722	-0.236258
1	1.482677	3.624271	-1.677785
1	-0.281176	3.666740	-1.629816
6	2.917013	2.351983	0.546950
1	2.925439	3.435831	0.383307
1	3.544226	2.139760	1.413646
1	3.385795	1.887744	-0.330395
1	0.001764	0.902209	1.799038
1	2.843836	1.150059	3.029798
1	1.316126	1.043119	3.919478
1	1.908762	-0.348331	3.010949

Product 2 (Prod2, ring closed product)

E_{SCF} = -855.877016076 Hartree

Singlet, neutral

6	-1.335471	0.297141	0.776613
6	-1.981278	1.580836	0.253541
6	-3.449130	1.792583	0.489554
1	-3.656068	1.932522	1.558317
1	-3.841181	2.664531	-0.038936
1	-4.019013	0.912694	0.166547
6	-1.122285	2.421142	-0.350709
6	-1.437068	3.772222	-0.926589
1	-0.991365	4.570554	-0.320060
1	-1.012046	3.865941	-1.934146
1	-2.510001	3.966890	-0.991717
6	0.313930	1.919705	-0.413588
1	0.623726	1.869204	-1.470470
6	1.294687	2.852112	0.326279
1	0.984682	2.981857	1.370071
1	2.312013	2.447381	0.327271
1	1.330703	3.845697	-0.134843
5	0.175050	0.486336	0.262197
6	2.511606	-0.588321	0.173457
6	3.061484	0.126022	-0.895912
6	4.422251	0.030671	-1.175060
1	4.832459	0.593386	-2.008773
6	5.251837	-0.787815	-0.410269
6	4.701665	-1.516818	0.642765
6	3.344918	-1.416316	0.934585
1	2.923031	-1.976642	1.766013
1	5.330931	-2.164508	1.246343
1	6.310776	-0.862257	-0.636579
1	2.420669	0.740784	-1.517772
6	-1.941620	-0.946881	0.142176
6	-2.251351	-2.101669	0.869564
1	-2.112659	-2.122244	1.946385
6	-2.756353	-3.240331	0.236229
1	-2.991289	-4.121365	0.827359
6	-2.965476	-3.247427	-1.138759
1	-3.360550	-4.131407	-1.630518
6	-2.665699	-2.101803	-1.878493
1	-2.826715	-2.090077	-2.953002
6	-2.160981	-0.971738	-1.245243
1	-1.937562	-0.080369	-1.829061
6	-1.384803	0.266985	2.315694
1	-1.000626	1.209779	2.719696
1	-2.408648	0.132209	2.687193
1	-0.772406	-0.541086	2.733306
7	1.139433	-0.511994	0.493244
1	0.814660	-1.332998	0.998659

Intermediate 3 (Ph migration from Int1)

E_{SCF} = -855.798569123 Hartree

Singlet, neutral

6	-1.646752	0.004182	0.801565
6	-2.539214	0.837739	-0.108147
6	-3.938045	0.381733	-0.393167
1	-4.547906	0.336936	0.521152
1	-4.455348	1.039286	-1.097237
1	-3.944099	-0.631438	-0.821919
6	-1.897693	1.956430	-0.533215
6	-2.483571	3.025716	-1.414684
1	-2.449006	4.001901	-0.914879
1	-1.907859	3.127565	-2.343191
1	-3.523024	2.824378	-1.684766
6	-0.495896	2.066860	-0.049556
6	0.371591	3.217675	-0.481011
1	-0.010540	4.186600	-0.128209
1	1.394566	3.119754	-0.101431
1	0.445616	3.292915	-1.575385
5	-0.319178	0.904295	0.775471
6	-1.253332	-1.330259	0.201126
6	-0.933861	-2.445195	0.991092
1	-1.103686	-2.418549	2.065067
6	-0.429270	-3.622027	0.422705
1	-0.194425	-4.468067	1.063406
6	-0.245300	-3.715112	-0.951544
1	0.138084	-4.628888	-1.395986
6	-0.577951	-2.618558	-1.756478
1	-0.447616	-2.678360	-2.833915
6	-1.067845	-1.449316	-1.189843
1	-1.301157	-0.589584	-1.814012
6	-2.267481	-0.112628	2.204082
1	-2.585463	0.880496	2.537662
1	-3.143194	-0.775982	2.210153
1	-1.567691	-0.500694	2.957577
7	0.958105	0.335078	1.538116
1	1.125212	0.864191	2.397312
6	2.189735	0.282128	0.748630
6	3.168904	1.246968	0.938761
6	2.334006	-0.733707	-0.190661
6	4.324285	1.200401	0.158593
1	3.028960	2.035683	1.674343
6	3.494942	-0.774360	-0.956418
1	1.545262	-1.470847	-0.328892
6	4.488596	0.191390	-0.786724
1	5.092750	1.954905	0.294361
1	3.618803	-1.563008	-1.691951
1	5.389167	0.156281	-1.391706
1	0.716664	-0.622861	1.827633

Product 3 (Prod3, Bisborole)

E_{SCF} = -1424.20745325 Hartree

Singlet, neutral

6	-2.744843	-2.444425	2.459307
6	-1.976970	-2.385551	1.173227
1	-0.912744	-2.168454	1.243961
6	-2.483823	-2.567264	-0.056817
6	-1.619006	-2.363109	-1.243821
6	-0.944972	-1.201076	-1.398907
5	-1.203987	0.067496	-0.495415
7	-0.085162	0.843616	-0.003041
5	1.214302	0.260228	0.403352
6	1.240849	-0.840783	1.526046
6	2.088069	-1.898485	1.545822
6	2.908995	-2.255964	0.366374
6	2.320960	-2.428396	-0.828579
1	1.235944	-2.353069	-0.867300
6	3.031298	-2.717274	-2.117305
1	4.056891	-3.062316	-1.959489
1	2.499877	-3.476639	-2.701540
1	3.078028	-1.809964	-2.735879
6	4.403213	-2.409480	0.567924
1	4.692196	-2.180637	1.598011
1	4.750600	-3.423575	0.338114
1	4.944142	-1.713152	-0.083133
6	2.212424	-2.806168	2.751385
1	2.352439	-2.243514	3.681110
1	1.297493	-3.402954	2.866986
1	3.043085	-3.508324	2.642152
6	0.366322	-0.557883	2.738840
1	0.028821	-1.469248	3.244336
1	0.914614	0.038042	3.483123
1	-0.524136	0.015130	2.457904
6	2.538784	0.944344	-0.109322
6	3.739411	0.868817	0.614430
1	3.753132	0.332959	1.561553
6	4.909296	1.467809	0.151196
1	5.823010	1.401528	0.736024
6	4.906002	2.149929	-1.064912
1	5.816986	2.614238	-1.432714
6	3.725713	2.241832	-1.803610
1	3.715018	2.778483	-2.748267
6	2.558403	1.655608	-1.321493
1	1.637918	1.754556	-1.893627
6	-0.197698	2.259506	0.146600
6	-0.794300	3.044661	-0.846884
6	-0.901116	4.422497	-0.690070
6	-0.395766	5.045051	0.451779
6	0.214421	4.272244	1.437215
6	0.307287	2.890174	1.289145
1	0.769028	2.289690	2.070503
1	0.615705	4.742859	2.330226
1	-0.474056	6.121567	0.569160
1	-1.373895	5.013709	-1.469133
1	-1.175414	2.563443	-1.744339
6	-2.686666	0.591227	-0.321474
6	-3.091526	1.266959	0.842284
1	-2.357092	1.485264	1.615783
6	-4.411946	1.666500	1.029794
1	-4.700729	2.175257	1.945525
6	-5.360989	1.426324	0.034379
1	-6.389382	1.749226	0.171709
6	-4.982016	0.771376	-1.135848
1	-5.714905	0.580995	-1.915509
6	-3.663063	0.346989	-1.298798
1	-3.384849	-0.191533	-2.203297
6	-0.043728	-0.969414	-2.598289
1	0.875491	-0.445789	-2.310927
1	0.248485	-1.895278	-3.104084
1	-0.546658	-0.331443	-3.339946
6	-1.533272	-3.512389	-2.228490
1	-2.223390	-4.316776	-1.959908
1	-1.755017	-3.199236	-3.254871
1	-0.522723	-3.941634	-2.228098
6	-3.935200	-2.925769	-0.300951
1	-4.229155	-3.849236	0.210631
1	-4.584142	-2.118047	0.058931
1	-4.139026	-3.050040	-1.368552
1	-2.231014	-3.064554	3.203033
1	-2.837857	-1.437388	2.889461
1	-3.755434	-2.838572	2.322919

PH_2Ph reaction

Intermediate 1 (adduct)

E_{SCF} = -1142.39033135 Hartree
Singlet, neutral

15	-0.019809	-0.223255	1.497999
5	0.957082	0.020152	-0.242691
6	0.229046	-1.154184	-1.064207
6	-0.798194	-0.584171	-1.747776
6	-1.818694	-1.261009	-2.620030
1	-1.778369	-0.882077	-3.648863
1	-1.675244	-2.343745	-2.657706
1	-2.835228	-1.069845	-2.250226
6	-0.865396	0.880703	-1.519667
6	-1.984768	1.698619	-2.100068
1	-2.049124	1.578637	-3.188360
1	-2.952869	1.382701	-1.685713
1	-1.859748	2.763846	-1.888376
6	0.130073	1.317831	-0.705133
6	0.307452	2.739708	-0.237793
1	0.833747	3.348367	-0.986025
1	-0.645889	3.244369	-0.032577
1	0.913151	2.786516	0.675920
6	0.606105	-2.607362	-1.055103
1	-0.010787	-3.219001	-1.721705
1	1.653858	-2.736395	-1.355356
1	0.525939	-3.044661	-0.047128
6	2.528021	0.020942	0.055960
6	3.171856	-1.054963	0.691565
1	2.586125	-1.917101	1.011157
6	4.547258	-1.062509	0.917952
1	5.012351	-1.912149	1.411200
6	5.325905	0.019060	0.506828
1	6.398637	0.018628	0.679005
6	4.715273	1.097930	-0.130016
1	5.313455	1.943315	-0.460186
6	3.336850	1.095266	-0.346125
1	2.878382	1.941977	-0.851826
6	-1.826962	-0.186626	1.375678
6	-2.518496	-1.312790	0.919966
1	-1.982481	-2.236152	0.712482
6	-3.894689	-1.246398	0.709816
1	-4.427759	-2.123266	0.354474
6	-4.581364	-0.056428	0.946573
1	-5.653062	-0.005755	0.778137
6	-3.893041	1.069448	1.398185
6	-2.517989	1.005906	1.610184
1	-1.980889	1.890231	1.945708
1	-4.424617	1.998722	1.579666
1	0.243207	0.730668	2.501177
1	0.239459	-1.403595	2.227861

TS1 (H-migration from Int1)

E_{SCF} = -1142.33678722 Hartree
Singlet, neutral

5	-0.920908	-0.025205	-0.117621
6	-0.598829	0.970854	1.089960
6	-1.298814	2.148411	0.936537
6	-1.262011	3.358360	1.830484
1	-0.560358	3.223934	2.656869
1	-0.964731	4.259290	1.280130
1	-2.248428	3.558934	2.266314
6	-2.099318	2.116497	-0.261592
6	-2.920672	3.296666	-0.684982
1	-3.606304	3.587168	0.119528
1	-2.281067	4.166510	-0.883288
1	-3.510833	3.091154	-1.579894
6	-1.899907	0.938171	-0.998058
6	-2.691801	0.525813	-2.212646
1	-3.000171	1.366334	-2.843330
1	-2.111149	-0.166771	-2.831166
1	-3.594694	-0.015296	-1.904774
6	0.298702	0.632473	2.240667
1	1.077028	-0.075353	1.937348
1	0.779704	1.498479	2.708338
1	-0.298649	0.122232	3.008767
6	-1.225987	-1.566372	0.127384
6	-0.212195	-2.533009	0.215468
1	0.824638	-2.230366	0.071569
6	-0.495215	-3.872779	0.481132
1	0.313946	-4.596077	0.542827
6	-1.814475	-4.284775	0.664000
1	-2.040174	-5.328105	0.866643
6	-2.841704	-3.345187	0.583731
1	-3.874070	-3.654537	0.726091
6	-2.544946	-2.008075	0.321309
1	-3.358795	-1.285993	0.271785
6	2.362112	0.306343	-0.689610
6	2.946223	1.200594	0.214588
1	2.371245	2.053679	0.569548
6	4.251780	1.003293	0.658832
1	4.693425	1.701789	1.363810
6	4.993374	-0.080927	0.190942
1	6.013343	-0.231327	0.532091
6	4.423511	-0.968114	-0.721923
6	3.114379	-0.777639	-1.159688
1	2.674023	-1.477882	-1.865890
1	4.997741	-1.812456	-1.092561
1	-0.693972	1.570526	-1.479269
15	0.632410	0.572596	-1.225215
1	0.611438	-0.152377	-2.434385

Product 1 (Prod1, ring opened product)

E_{SCF} = -1142.38487989 Hartree
Singlet, neutral

6	2.150715	1.422692	2.770914
6	1.144984	1.548719	1.667040
6	1.331057	2.093736	0.451225
6	0.281899	1.965360	-0.591479
6	-0.243699	0.750416	-0.869959
6	-1.309982	0.589442	-1.939232
1	-1.005432	1.089499	-2.866813
1	-1.491960	-0.463661	-2.175103
1	-2.272826	1.017109	-1.629080
5	0.272696	-0.537304	-0.149384
15	-0.911833	-1.588436	0.966154
1	-0.877219	-2.818233	0.266902
6	-2.590176	-1.013704	0.506522
6	-3.031117	0.217327	1.010446
6	-4.284690	0.719799	0.668931
6	-5.128652	-0.011877	-0.166194
1	-6.107947	0.376345	-0.430132
6	-4.710035	-1.249746	-0.652638
6	-3.450030	-1.744953	-0.320871
1	-3.127831	-2.702699	-0.722963
1	-5.362479	-1.829513	-1.299659
1	-4.604704	1.681206	1.060924
1	-2.383990	0.794934	1.667872
6	1.742570	-1.051376	-0.320193
6	2.327294	-1.976089	0.564586
1	1.756221	-2.335445	1.419140
6	3.633080	-2.425726	0.388166
1	4.065503	-3.130190	1.093192
6	4.384461	-1.972574	-0.696863
1	5.401469	-2.326872	-0.840743
6	3.826040	-1.064380	-1.595656
1	4.406359	-0.711402	-2.443832
6	2.524365	-0.606673	-1.401837
1	2.097993	0.110349	-2.100427
6	-0.145765	3.218146	-1.324459
1	0.109323	4.119743	-0.759993
1	0.330092	3.294557	-2.311491
1	-1.228317	3.218670	-1.488347
6	2.611414	2.770527	0.024489
1	2.410213	3.575751	-0.689022
1	3.167221	3.195629	0.863118
1	3.260724	2.043652	-0.482892
1	0.161894	1.130816	1.884859
1	3.108681	1.886522	2.526866
1	1.777683	1.862003	3.702960
1	2.340938	0.359907	2.971656

Product 2 (Prod2, ring closed product)

E_{SCF} = -1142.4027099 Hartree
Singlet, neutral

6	-1.322852	0.425012	0.723792
6	-1.664154	1.863314	0.321486
6	-2.970294	2.448204	0.775400
1	-2.991517	2.548050	1.868237
1	-3.159244	3.436739	0.350404
1	-3.803935	1.791451	0.499005
6	-0.695032	2.472967	-0.384361
6	-0.698814	3.887073	-0.890483
1	0.007671	4.509670	-0.327618
1	-0.381144	3.916582	-1.940296
1	-1.682072	4.358224	-0.821005
6	0.534564	1.605752	-0.624992
1	0.762066	1.544489	-1.702662
6	1.790252	2.172079	0.078365
1	1.641756	2.221287	1.163901
1	2.672837	1.555590	-0.114993
1	2.005340	3.187876	-0.271748
5	0.062394	0.212682	-0.040141
6	2.636378	-1.155126	-0.146962
6	3.400256	-0.906501	-1.293210
6	4.750577	-0.572972	-1.190389
1	5.326838	-0.374195	-2.089538
6	5.360935	-0.506908	0.060560
6	4.614255	-0.776886	1.207824
6	3.261158	-1.092093	1.104967
1	2.682006	-1.277457	2.006712
1	5.084011	-0.730888	2.186340
1	6.413608	-0.252733	0.142158
1	2.934151	-0.972204	-2.273786
6	-2.348996	-0.580205	0.219285
6	-2.785823	-1.670150	0.980353
1	-2.431613	-1.802967	1.997923
6	-3.683155	-2.601226	0.453570
1	-4.007324	-3.437661	1.066641
6	-4.163355	-2.461258	-0.844907
1	-4.861740	-3.185657	-1.253356
6	-3.739329	-1.377695	-1.615322
1	-4.106635	-1.253562	-2.630246
6	-2.844317	-0.452971	-1.088417
1	-2.522691	0.392717	-1.694008
6	-1.092886	0.336950	2.246716
1	-0.403165	1.124381	2.569156
1	-2.033647	0.466856	2.796507
1	-0.661490	-0.625581	2.542871
15	0.840449	-1.494635	-0.353984
1	0.561012	-2.129060	0.880217

Intermediate 3 (Ph migration from Int1)

E_{SCF} = -1142.3609863 Hartree

Singlet, neutral

6	-1.805079	0.263162	0.791666
6	-2.433102	1.366557	-0.059423
6	-3.893719	1.297994	-0.383550
1	-4.510574	1.393403	0.521219
1	-4.205910	2.081756	-1.078575
1	-4.144550	0.328053	-0.834699
6	-1.534923	2.324571	-0.401737
6	-1.816934	3.568548	-1.199028
1	-1.602621	4.467585	-0.607725
1	-1.179374	3.617691	-2.090456
1	-2.857180	3.627048	-1.527743
6	-0.173260	2.035776	0.105859
6	0.968579	2.962107	-0.202035
1	0.776347	3.979287	0.166268
1	1.904598	2.624249	0.255438
1	1.146680	3.053311	-1.283947
5	-0.287096	0.795828	0.844201
6	-1.860562	-1.082206	0.084681
6	-2.231842	-2.269171	0.724447
1	-2.552573	-2.250723	1.761886
6	-2.212123	-3.494658	0.047845
1	-2.510359	-4.399136	0.571650
6	-1.823854	-3.557094	-1.284522
1	-1.811819	-4.506708	-1.811514
6	-1.455207	-2.377899	-1.941057
1	-1.155182	-2.408928	-2.985293
6	-1.472812	-1.164777	-1.265325
1	-1.188206	-0.246504	-1.776849
6	-2.469383	0.246038	2.179456
1	-2.435657	1.252540	2.609208
1	-3.520251	-0.070008	2.126615
1	-1.958072	-0.428593	2.876847
15	1.129061	-0.265137	1.497413
1	1.627837	-0.089901	2.805698
6	2.667909	-0.263104	0.525250
6	3.901949	-0.507064	1.135196
6	2.600016	-0.020724	-0.849434
6	5.065208	-0.518302	0.369353
1	3.958909	-0.685536	2.206512
6	3.766411	-0.036720	-1.611122
1	1.636800	0.192763	-1.307921
6	4.996546	-0.285214	-1.003925
1	6.023364	-0.705003	0.844767
1	3.713755	0.152134	-2.678999
1	5.904298	-0.292220	-1.600054
1	0.736388	-1.615557	1.579900

Intermediate 2 (H migration from Int1)

E_{SCF} = -1142.39255562 Hartree

Singlet, neutral

5	-0.914661	0.112565	-0.034088
1	0.319289	-0.922736	-1.753752
6	-0.279366	1.344126	0.643581
6	0.879309	1.778695	-0.090445
6	1.798923	2.875582	0.370458
1	1.295554	3.850296	0.357602
1	2.138474	2.706229	1.399106
1	2.688952	2.946935	-0.260250
6	1.034194	1.021744	-1.223636
6	2.200311	1.100290	-2.159091
1	2.432175	2.133867	-2.438684
1	3.096531	0.681778	-1.677808
1	2.013162	0.527225	-3.071472
6	-0.089274	0.047637	-1.439354
6	-1.000546	0.549723	-2.583593
1	-0.449015	0.667866	-3.524471
1	-1.817310	-0.159488	-2.748344
1	-1.447293	1.516516	-2.325359
6	-0.752052	2.101465	1.845365
1	0.056277	2.339591	2.547672
1	-1.164231	3.062895	1.505362
1	-1.546313	1.569566	2.376412
6	-2.467621	-0.236421	0.047878
6	-2.944832	-1.553247	-0.046844
1	-2.229528	-2.373116	-0.094416
6	-4.308049	-1.840852	-0.070956
1	-4.644323	-2.871784	-0.145432
6	-5.241474	-0.806616	0.006253
1	-6.305407	-1.026650	-0.007777
6	-4.797071	0.510436	0.101883
1	-5.514903	1.324629	0.159927
6	-3.428534	0.784124	0.120238
1	-3.100345	1.821164	0.181390
15	0.121321	-1.072648	1.376520
6	1.858557	-1.106296	0.830398
6	2.852338	-0.255989	1.338699
6	2.221307	-2.024729	-0.166761
6	4.160428	-0.316704	0.865590
1	2.594654	0.462383	2.113752
6	3.527062	-2.085023	-0.648967
1	1.470596	-2.705676	-0.563184
6	4.500354	-1.228338	-0.135753
1	4.914689	0.349941	1.274705
1	3.785446	-2.803274	-1.421824
1	5.519810	-1.274664	-0.507806
1	0.302763	-0.254243	2.517620

Product 3 (Prod3, bisborole)

E_{SCF} = -1710.69376701 Hartree

Singlet, neutral

6	-4.021670	-0.805726	2.867939
6	-3.153405	-1.474188	1.847831
1	-2.080760	-1.333714	1.975977
6	-3.560431	-2.176268	0.778608
6	-2.574319	-2.646286	-0.224124
6	-1.650328	-1.811772	-0.761592
5	-1.634185	-0.285713	-0.407338
15	-0.000009	0.539601	0.000346
5	1.634132	-0.285802	0.407667
6	1.650257	-1.811913	0.761735
6	2.574047	-2.646456	0.223987
6	3.560142	-2.176431	-0.778810
6	3.153038	-1.474282	-1.847950
1	2.080379	-1.333683	-1.975860
6	4.021001	-0.805868	-2.868355
1	5.061723	-1.132749	-2.819184
1	3.649868	-0.980015	-3.883316
1	4.011576	0.279718	-2.699793
6	5.010464	-2.461016	-0.470653
1	5.124037	-3.395607	0.086445
1	5.629654	-2.526936	-1.367922
1	5.410921	-1.656659	0.160390
6	2.625184	-4.113818	0.597190
1	3.005609	-4.266165	1.615268
1	1.621506	-4.552576	0.564174
1	3.259382	-4.680644	-0.088586
6	0.639260	-2.363960	1.749421
1	-0.157750	-2.929439	1.246537
1	1.114255	-3.040607	2.468618
1	0.157094	-1.562599	2.315183
6	2.923510	0.604216	0.538433
6	3.869270	0.301426	1.531569
1	3.695440	-0.551655	2.183350
6	5.023633	1.064233	1.694261
1	5.733232	0.814513	2.477944
6	5.270146	2.140554	0.846177
1	6.172499	2.733275	0.964309
6	4.353296	2.453161	-0.156517
1	4.541133	3.288586	-0.824582
6	3.191804	1.701391	-0.297778
1	2.480667	1.963986	-1.077809
6	0.000152	2.359479	0.000081
6	-0.560246	3.071455	-1.067662
6	-0.568388	4.463009	-1.062275
6	0.000497	5.162142	-0.000330
6	0.569206	4.463180	1.061822
6	0.560718	3.071630	1.067619
1	1.002981	2.530212	1.899296
1	1.014860	5.001432	1.892820
1	0.000632	6.247902	-0.000489
1	-1.013908	5.001127	-1.893432
1	-1.002639	2.529903	-1.899184
6	-2.923437	0.604477	-0.538120
6	-3.191583	1.701764	0.297990
1	-2.480437	1.964302	1.078032
6	-4.352943	2.453721	0.156619
1	-4.540658	3.289238	0.824603
6	-5.269816	2.141179	-0.846072
1	-6.172059	2.734050	-0.964287
6	-5.023466	1.064727	-1.694041
1	-5.733090	0.815048	-2.477716
6	-3.869234	0.301749	-1.531252
1	-3.695534	-0.551429	-2.182940
6	-0.639285	-2.363761	-1.749250
1	-0.157092	-1.562351	-2.314924
1	0.157705	-2.929259	-1.246368
1	-1.114248	-3.040337	-2.468529
6	-2.625721	-4.113562	-0.597626
1	-3.260158	-4.680364	0.087952
1	-3.006049	-4.265615	-1.615785
1	-1.622153	-4.552557	-0.564558
6	-5.010832	-2.460612	0.470479
1	-5.629530	-2.528934	1.367926
1	-5.411909	-1.654857	-0.158389
1	-5.124365	-3.393876	-0.088832
1	-3.650525	-0.979245	3.882998
1	-4.012756	0.279794	2.698874
1	-5.062243	-1.133115	2.818823