Synthesis, structure and DFT calculations of 1,2-*N*-substituted *o*-carboranes

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Electronic Supplementary Information

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(1) NMR Spectra

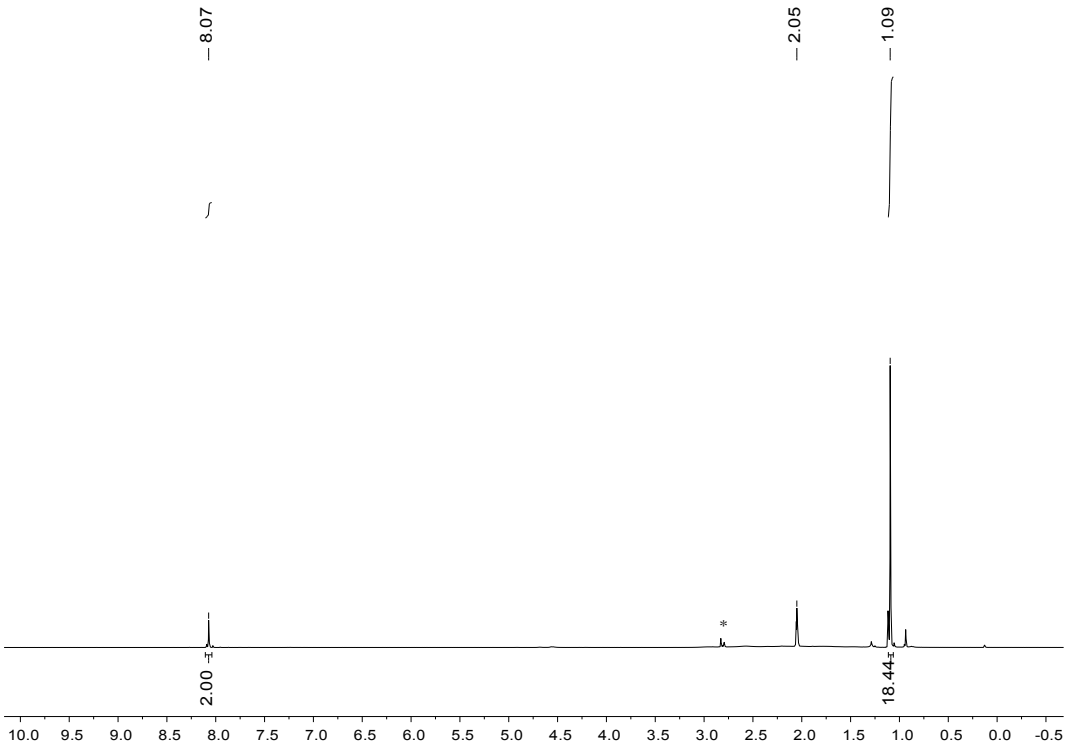

Fig. S1. ^{1}H NMR (Acetone-D6, 400.13 MHz) spectrum of Compound **2a**. (*:H_2O)

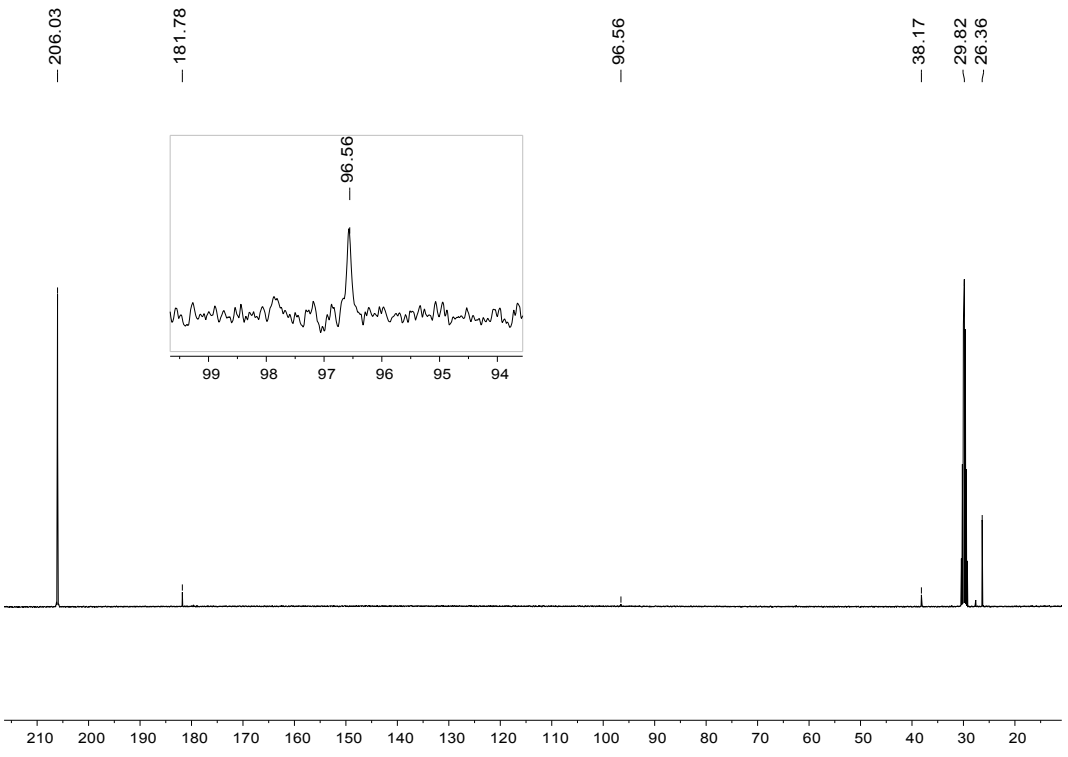

Fig. S2. $^{13}C\{^{1}H\}$ NMR (Acetone-D_6, 100.62 MHz) spectrum of Compound **2a**.

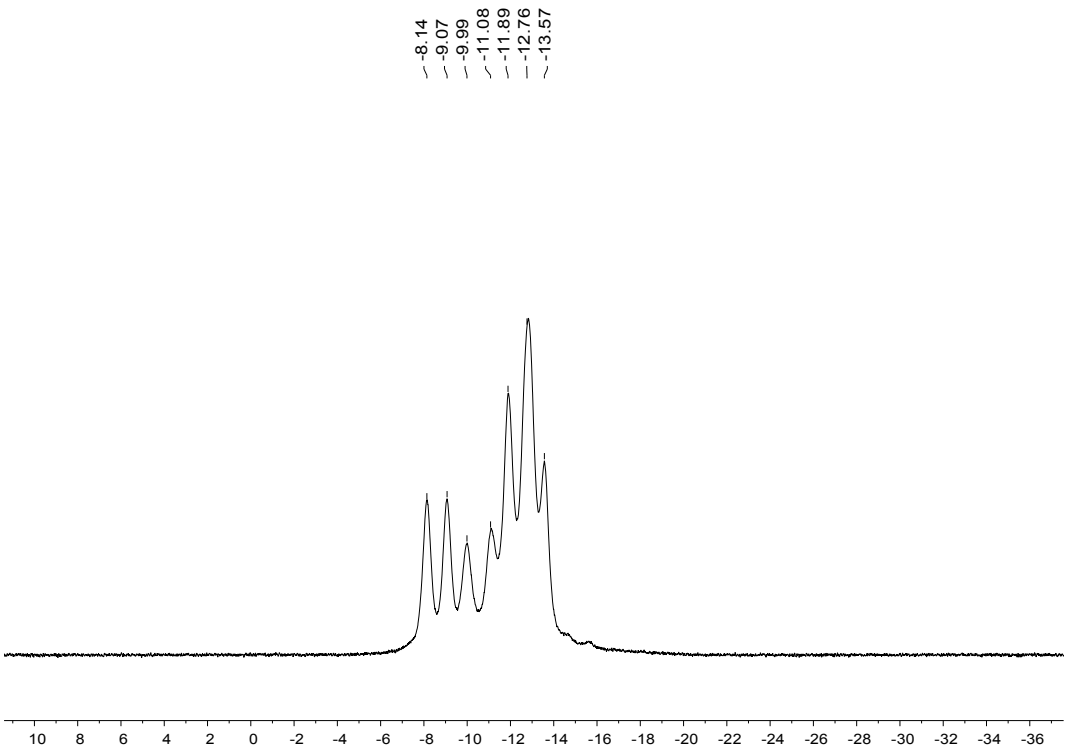

Fig. S3. ^{11}B NMR (Acetone-D_6, 160.46 MHz) spectrum of Compound **2a**.

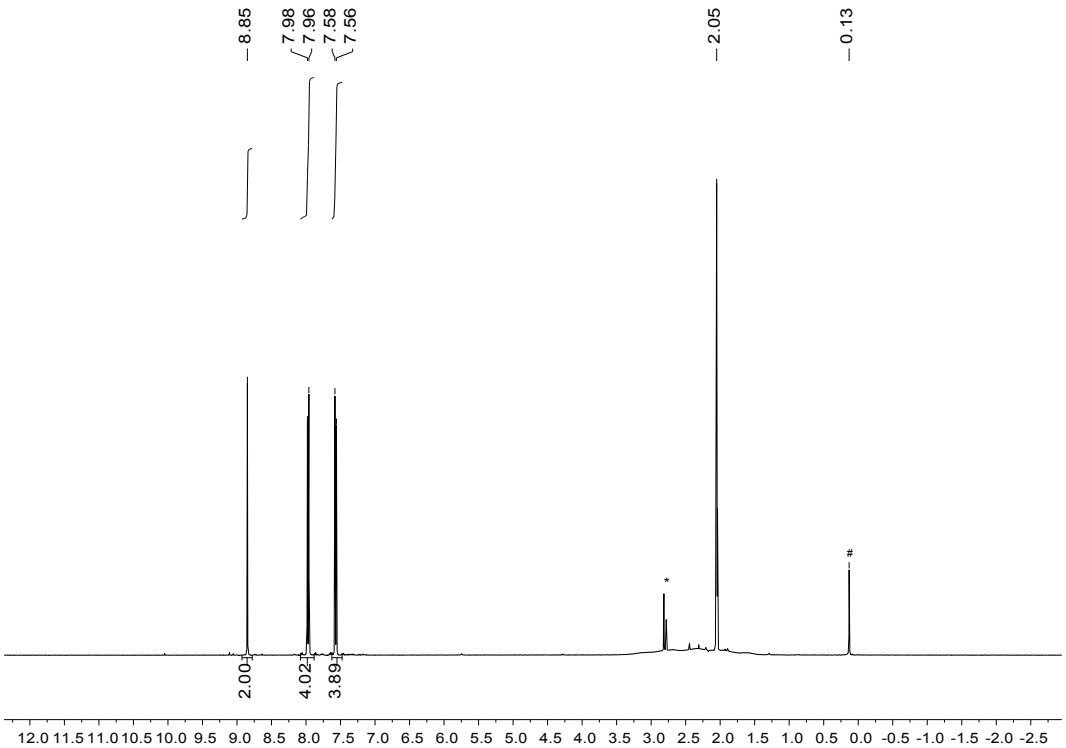

Fig. S4. ^{1}H NMR (Acetone-D_6, 400.13 MHz) spectrum of Compound **2b**. (*:H_2O; $^{\#}$: TMS)

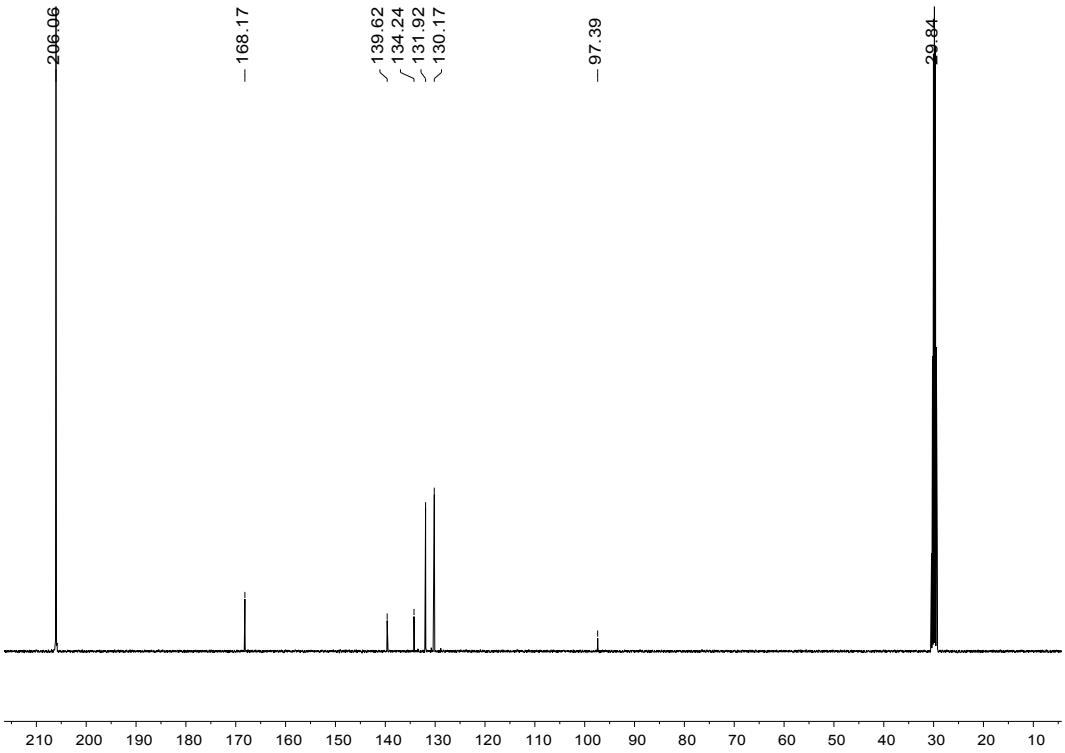

Fig. S5. $^{13}C\{^{1}H\}$ NMR (Acetone-D_6, 100.62 MHz) spectrum of Compound **2b**.

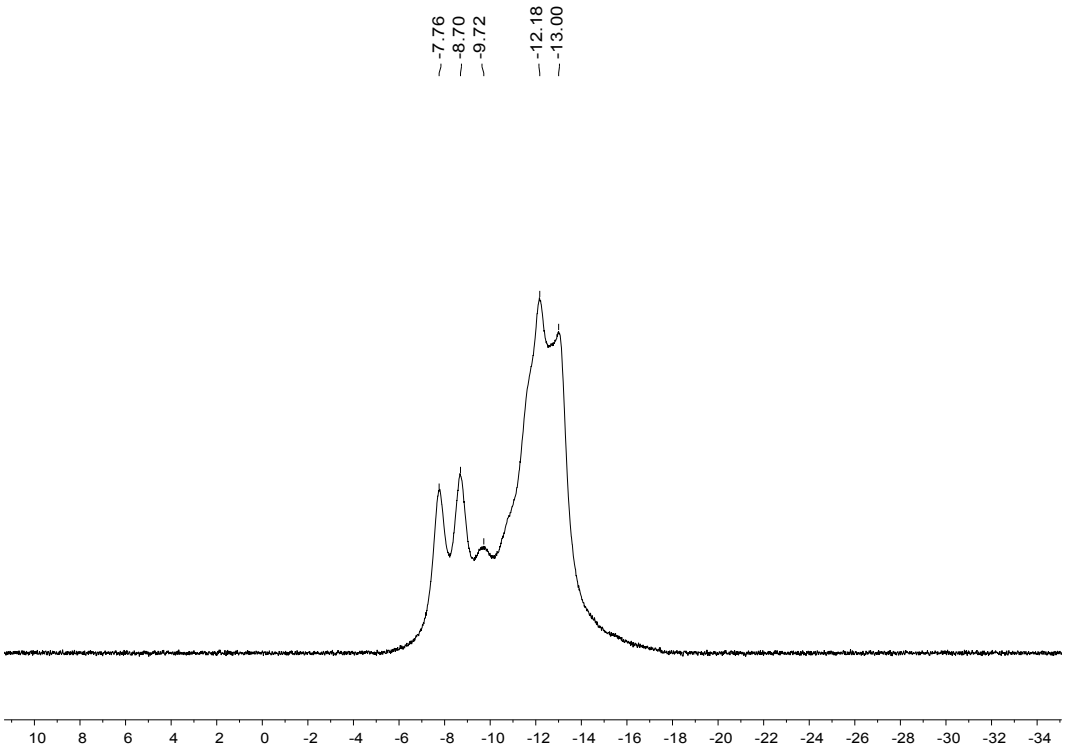

Fig. S6. ^{11}B NMR (Acetone-D_6, 160.46 MHz) spectrum of Compound **2b**.

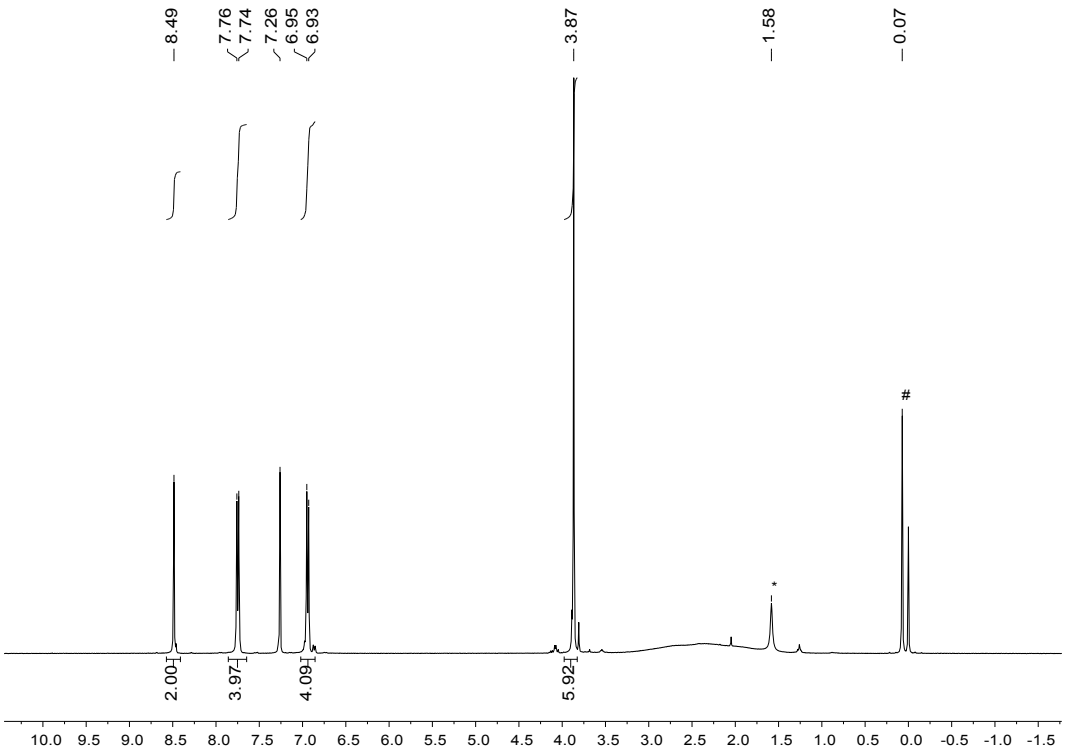

Fig. S7. ^{1}H NMR ($CDCl_3$, 400.13 MHz) spectrum of Compound **2c**. (*:H_2O; #: greese)

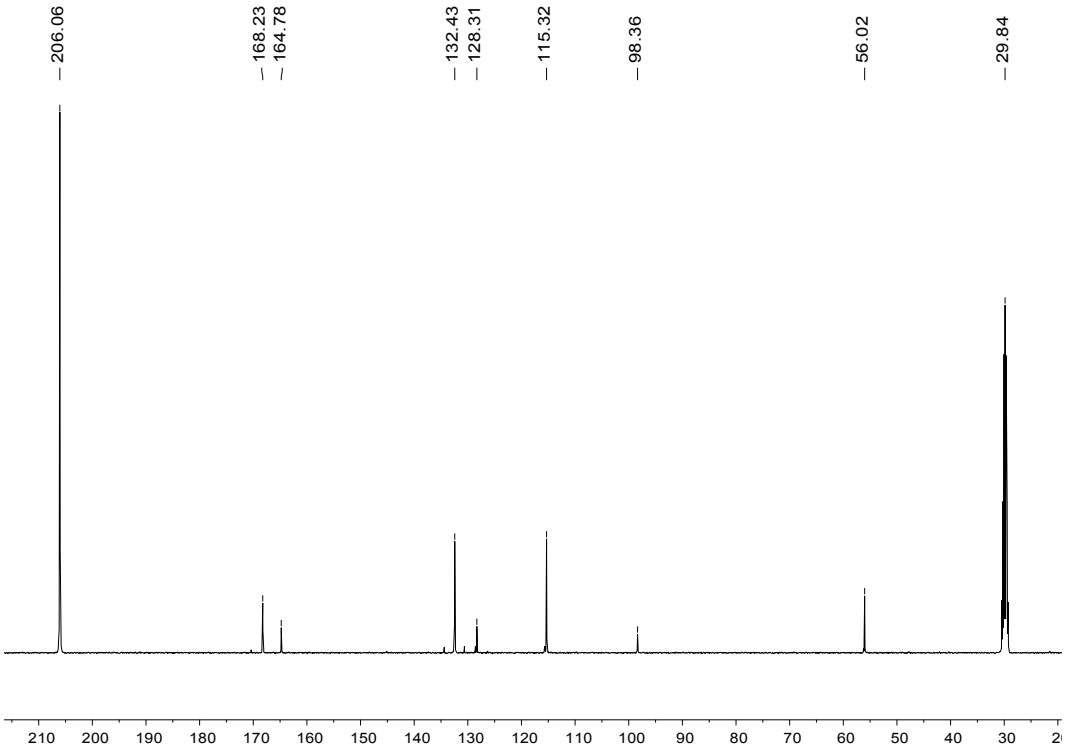

Fig. S8. $^{13}C\{^{1}H\}$ NMR (Acetone-D_6, 100.62 MHz) spectrum of Compound **2c**.

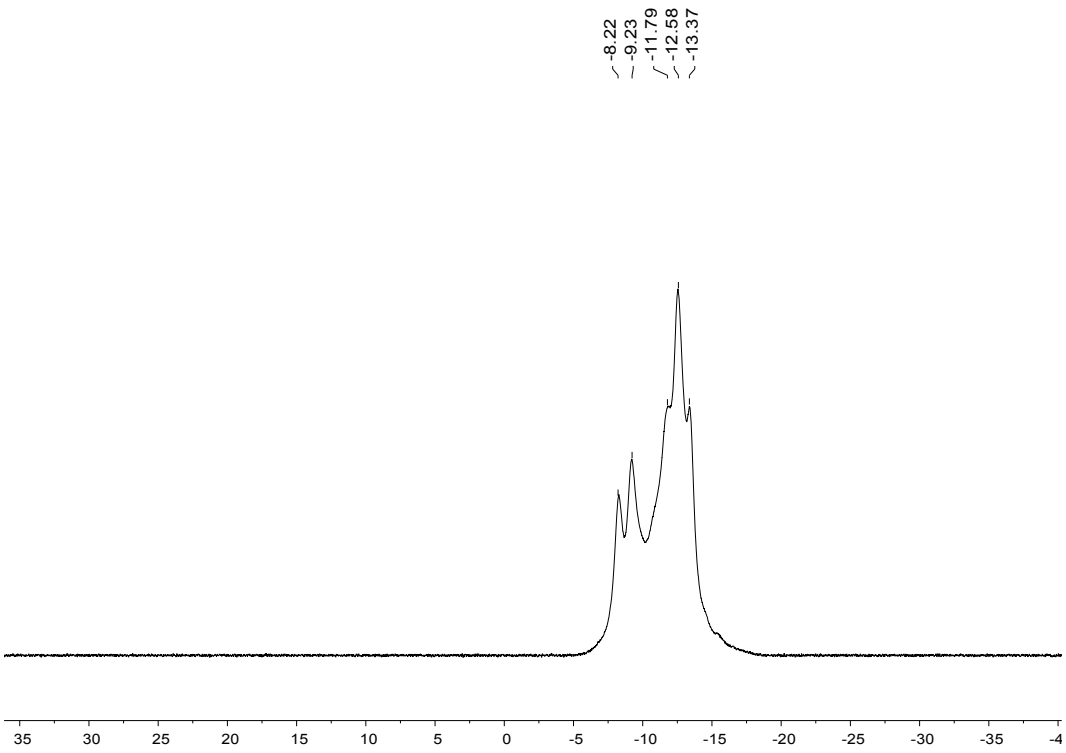

Fig. S9. ^{11}B NMR (Acetone-D_6, 160.46 MHz) spectrum of Compound **2c**.

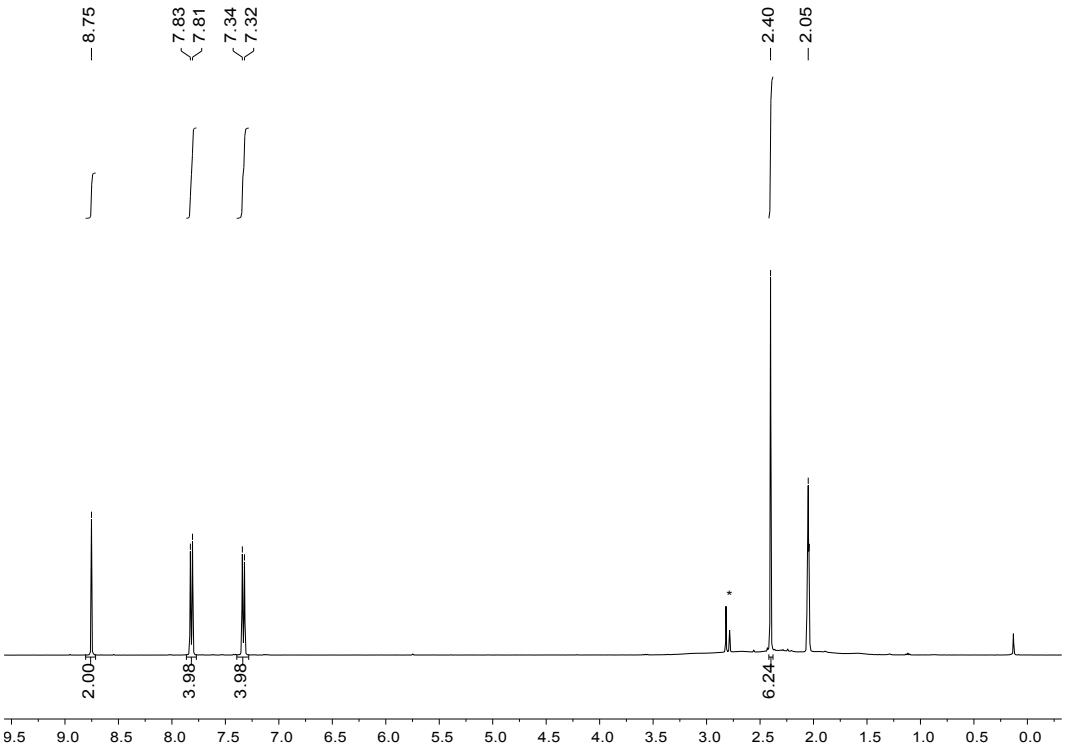

Fig. S10. ^{1}H NMR (Acetone-D_6, 400.13 MHz) spectrum of Compound **2d**. (*:H_2O)

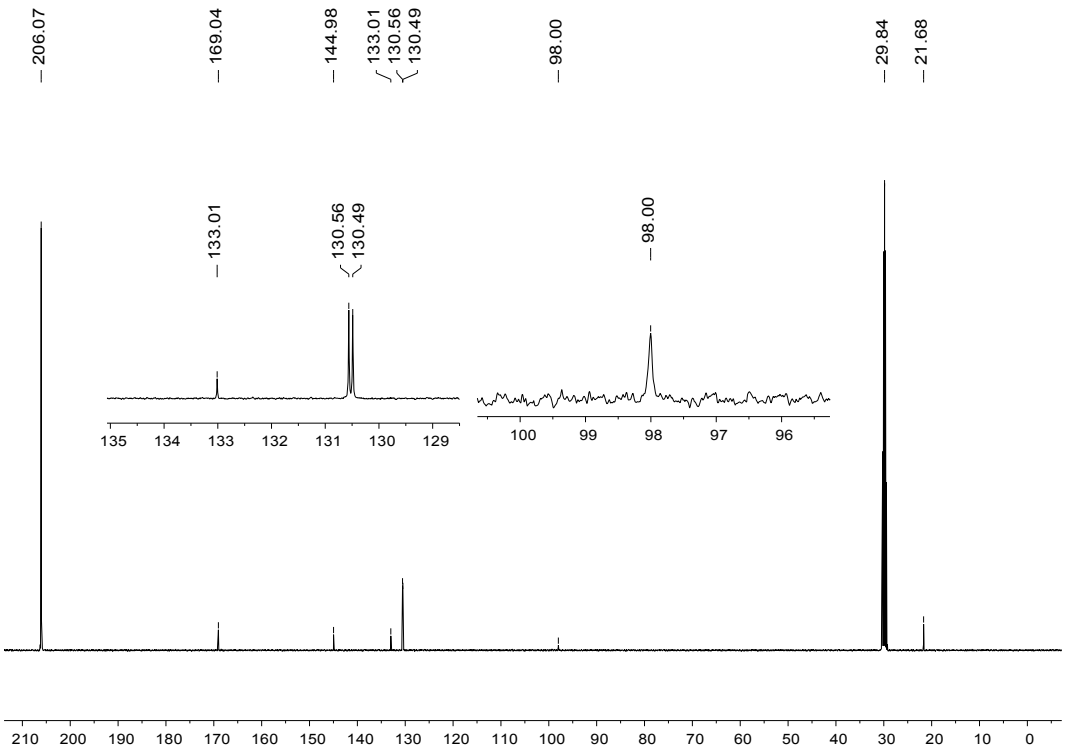

Fig. S11. $^{13}C\{^{1}H\}$ NMR (Acetone-D_6, 100.62 MHz) spectrum of Compound **2d**.

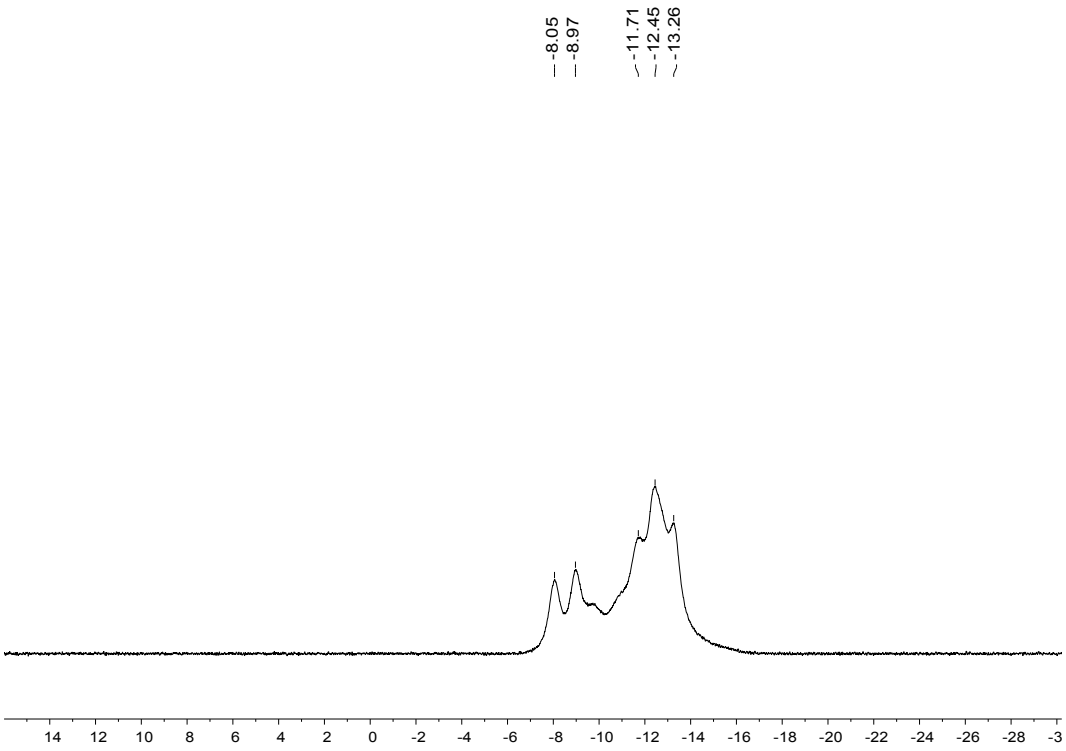

Fig. S12. ^{11}B NMR (Acetone-D_6, 160.46 MHz) spectrum of Compound **2d**.

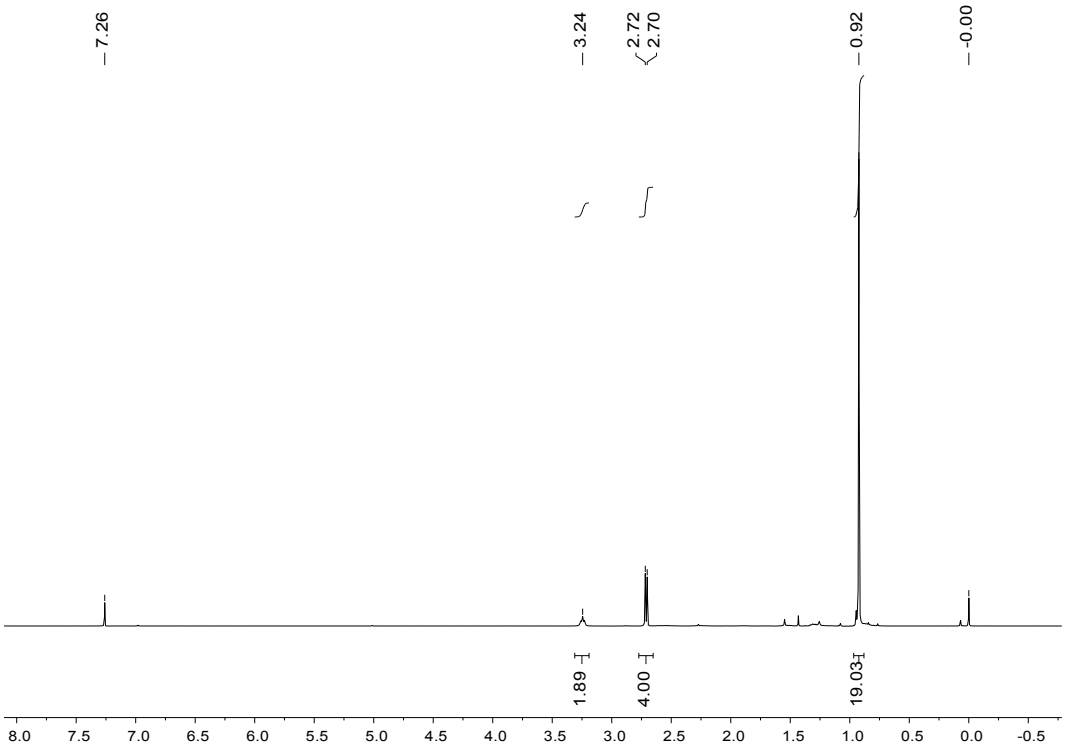

Fig. S13. ^{1}H NMR ($CDCl_3$, 400.13 MHz) spectrum of Compound **3a**.

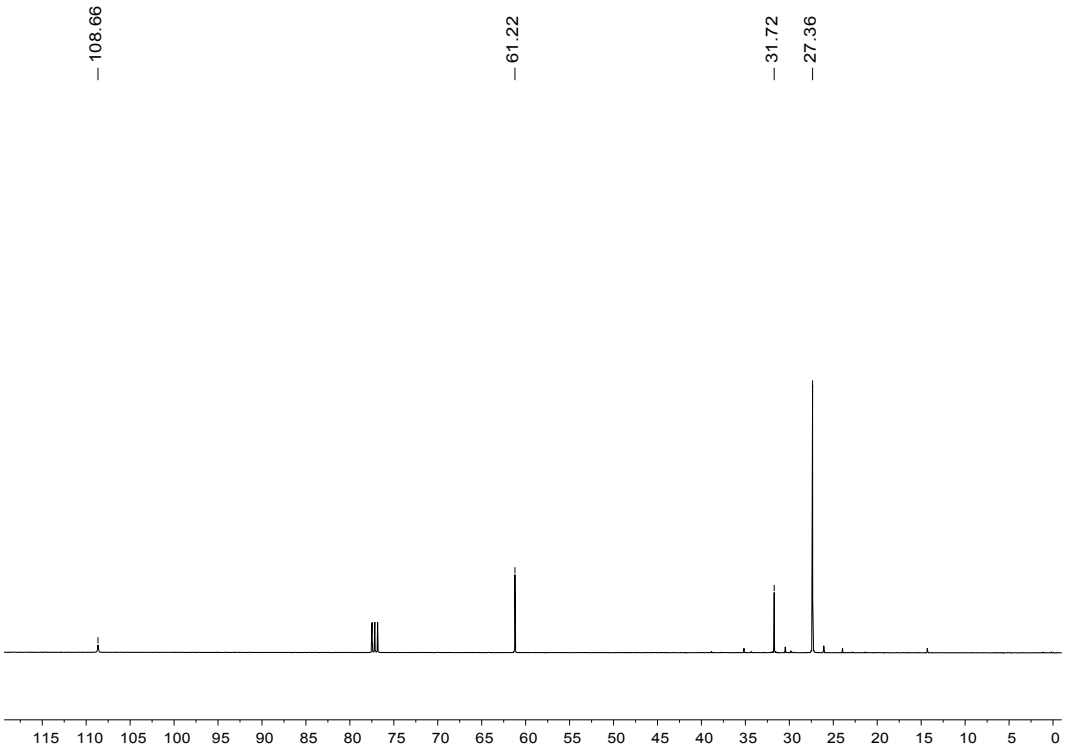

Fig. S14. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 100.62 MHz) spectrum of Compound **3a**.

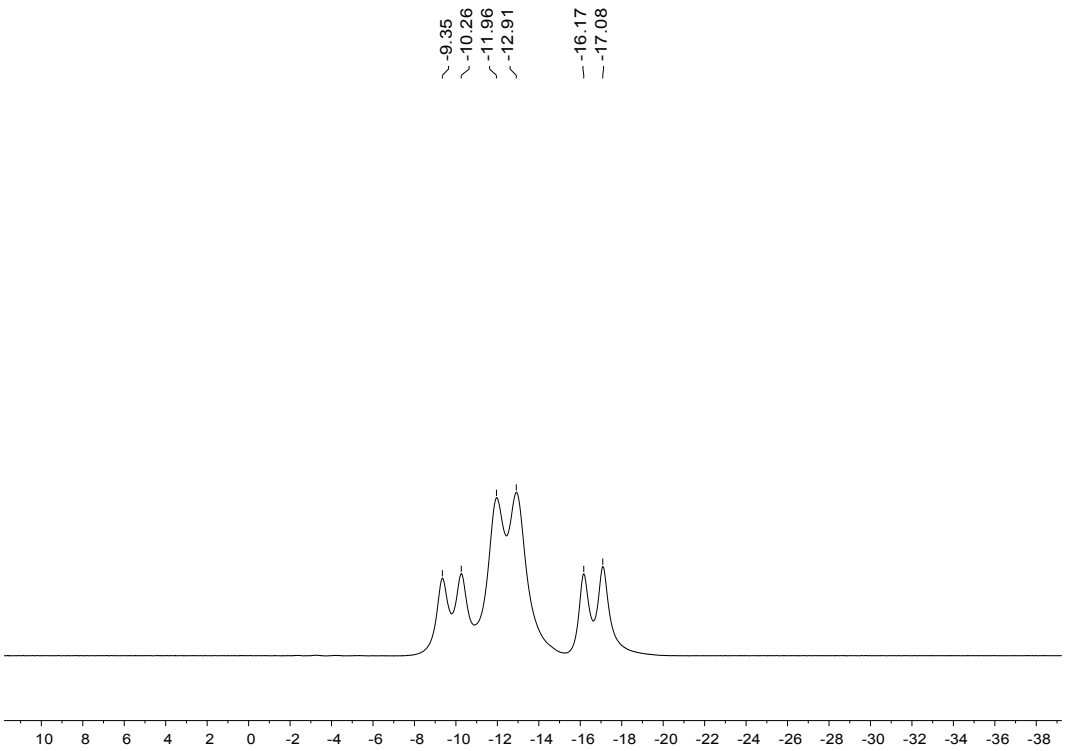

Fig. S15. ^{11}B NMR ($CDCl_3$, 160.46 MHz) spectrum of Compound **3a**.

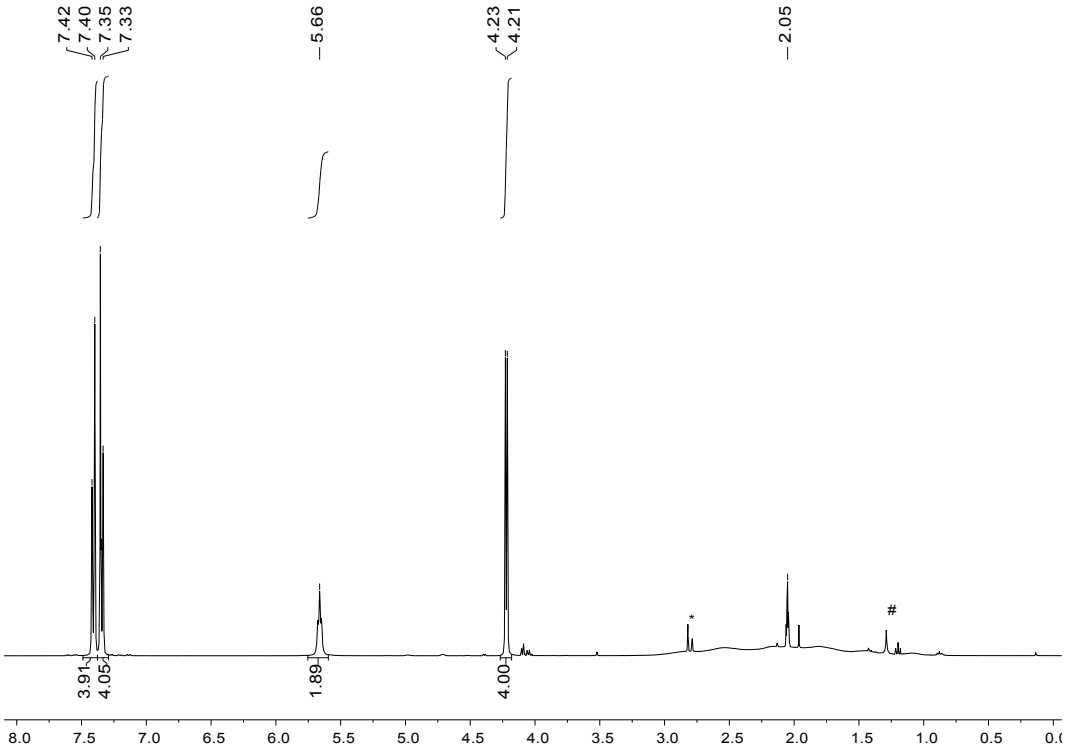

Fig. S16. ^1H NMR (Acetone-D_6, 400.13 MHz) spectrum of Compound **3b**. (*:H_2O; #:Hexane)

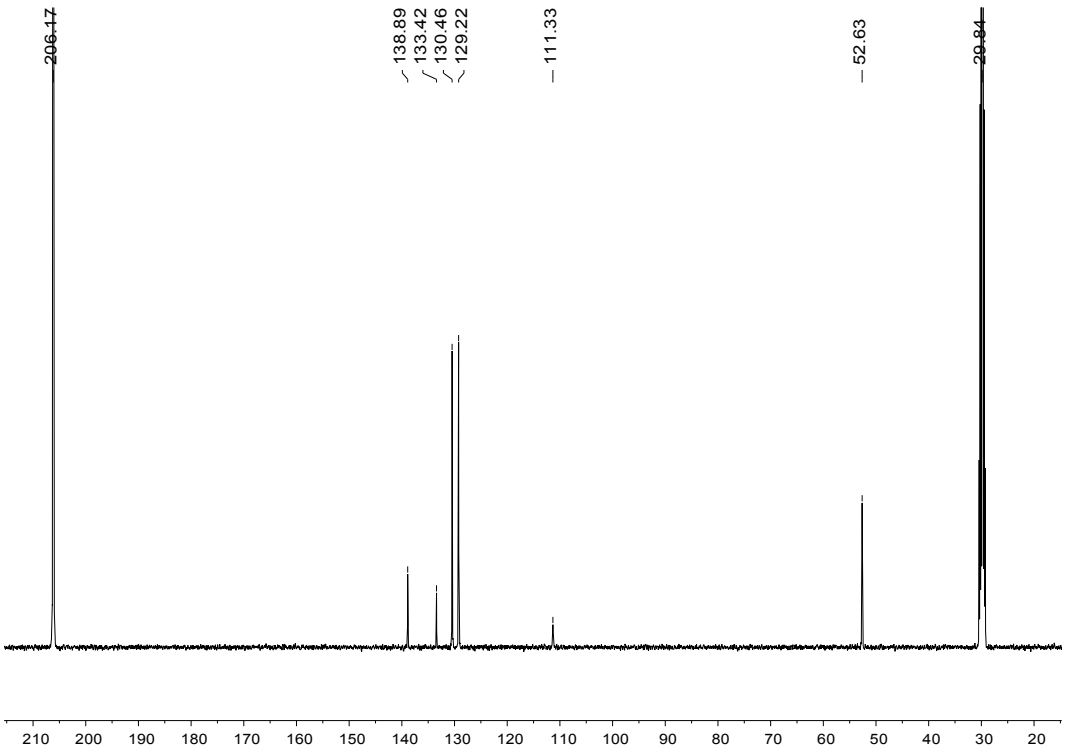

Fig. S17. $^{13}C\{^{1}H\}$ NMR (Acetone-D_6, 100.62 MHz) spectrum of Compound **3b**.

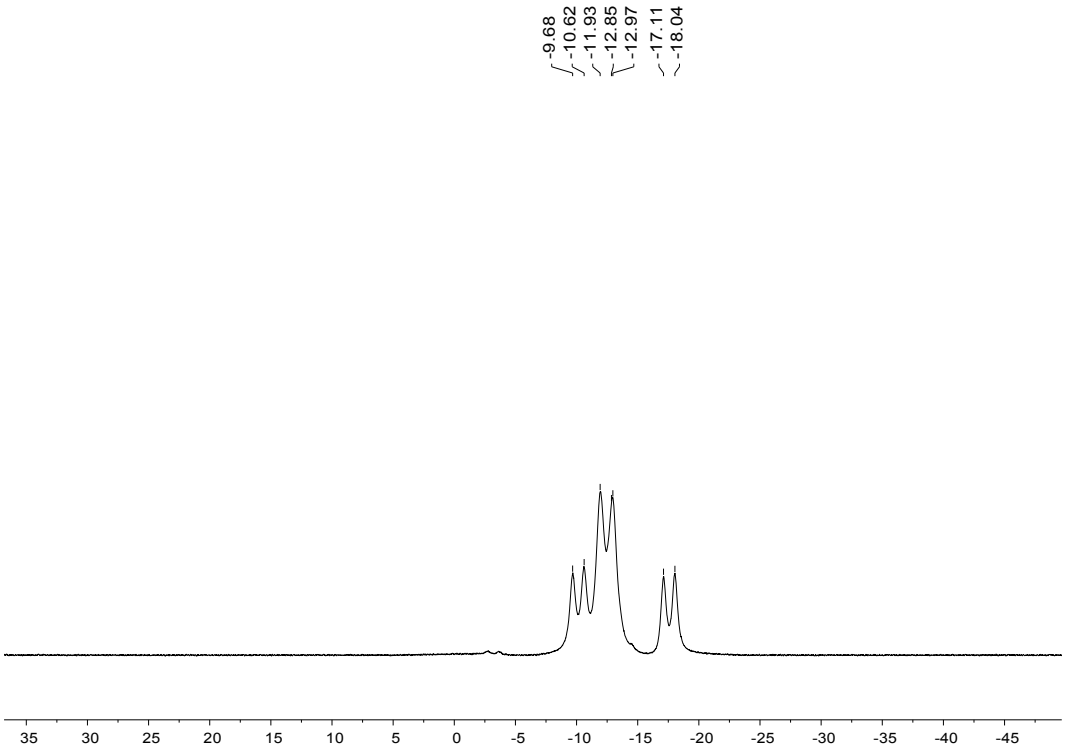

Fig. S18. ^{11}B NMR (Acetone-D_6, 160.46 MHz) spectrum of Compound **3b**.

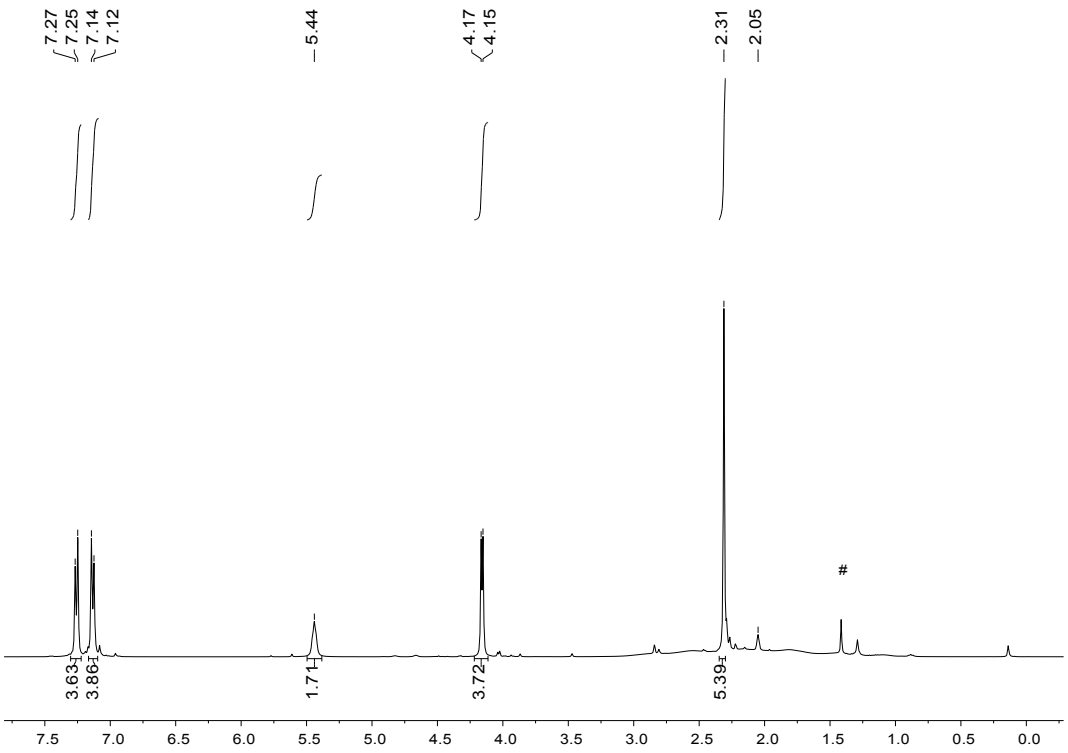

Fig. S19. ^{1}H NMR (Acetone-D_6, 400.13 MHz) spectrum of Compound **3c**. (#:Hexane)

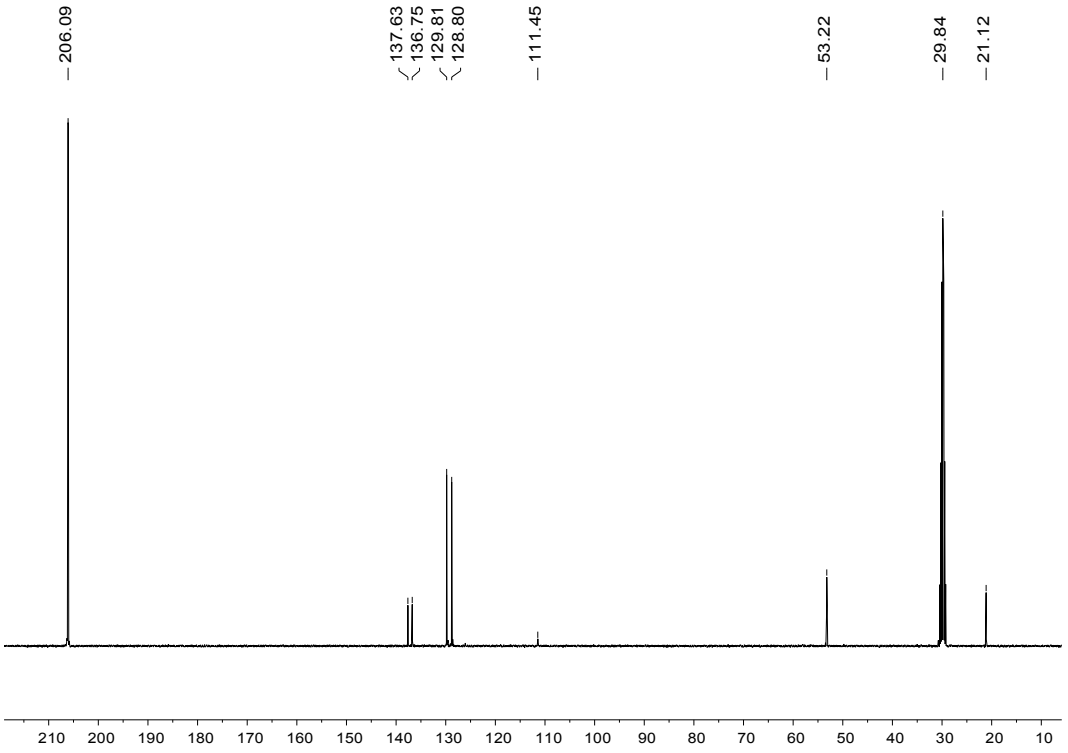

Fig. S20. $^{13}C\{^{1}H\}$ NMR (Acetone-D_6, 100.62 MHz) spectrum of Compound **3c**.

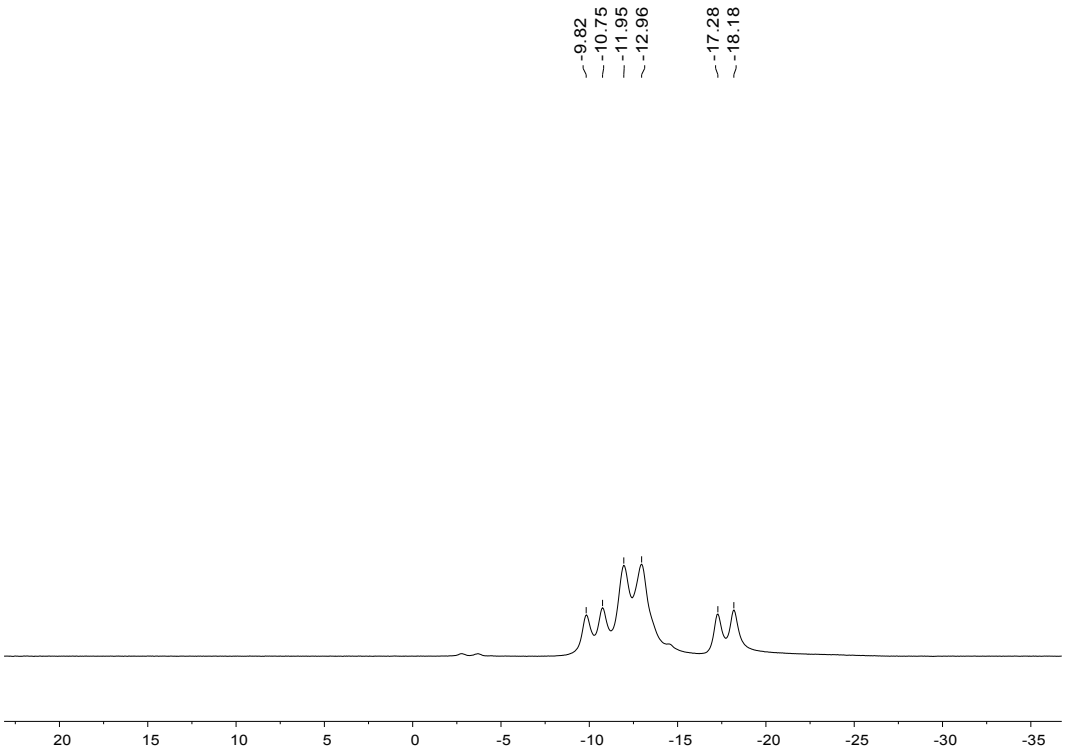

Fig. S21. ^{11}B NMR (Acetone-D_6, 160.46 MHz) spectrum of Compound **3c**.

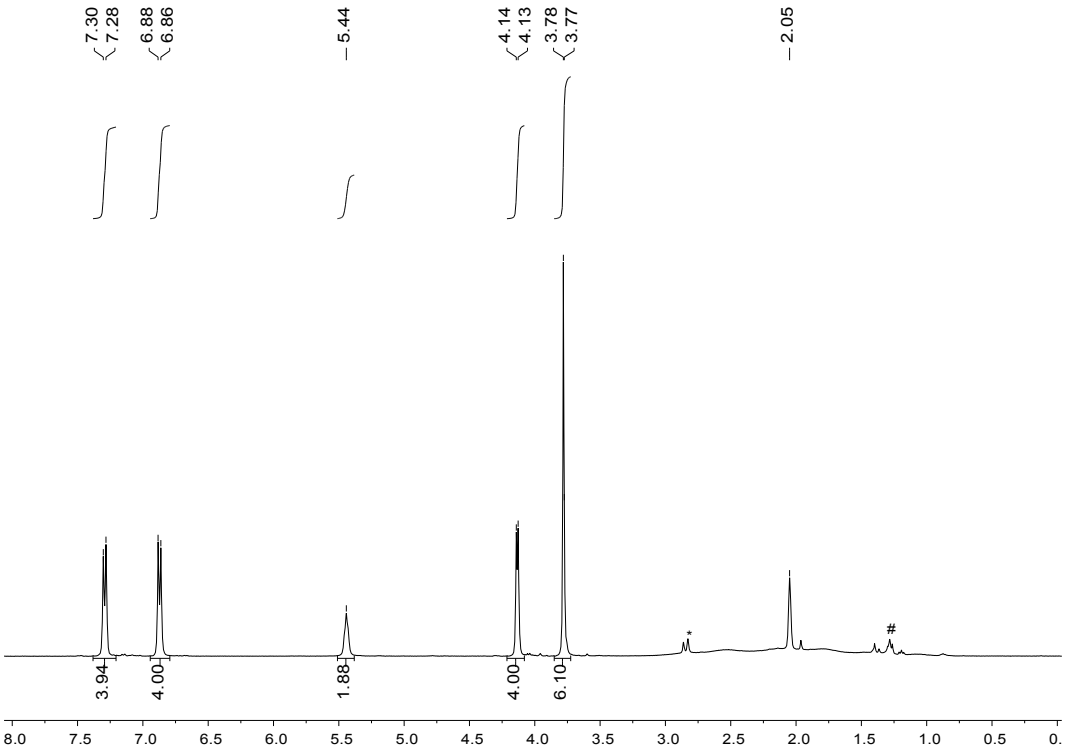

Fig. S22. ^{1}H NMR (Acetone-D_6, 400.13 MHz) spectrum of Compound **3d**. (*:H_2O; #:Hexane)

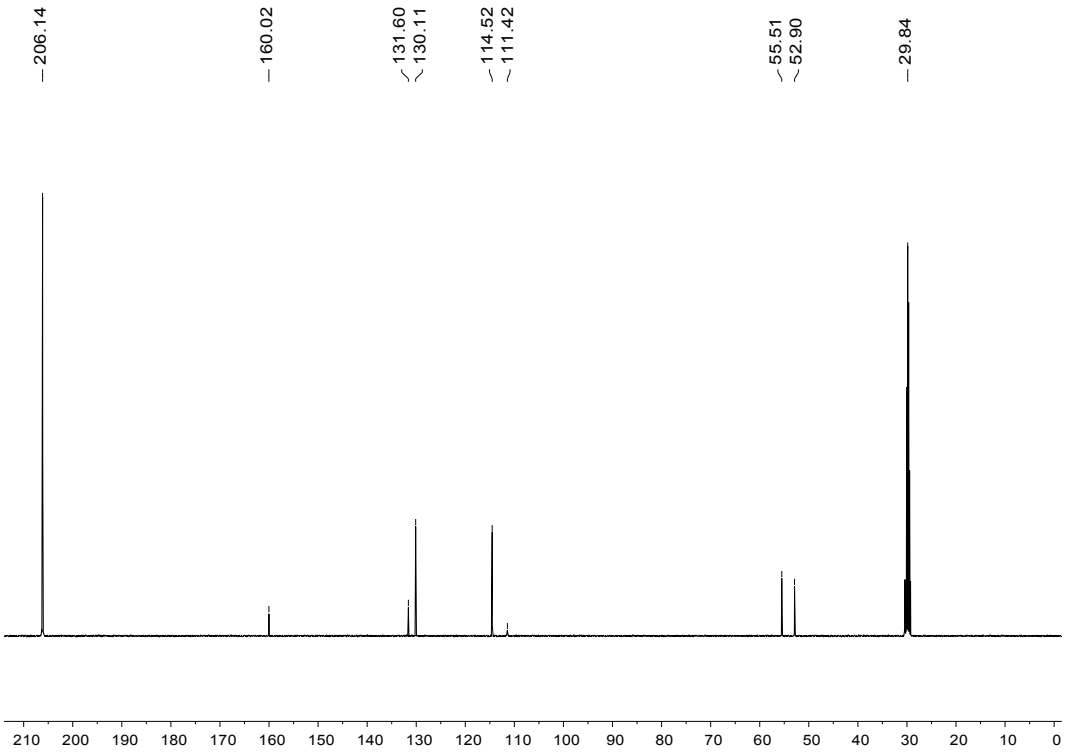

Fig. S23. $^{13}C\{^{1}H\}$ NMR (Acetone-D_6, 100.62 MHz) spectrum of Compound **3d**.

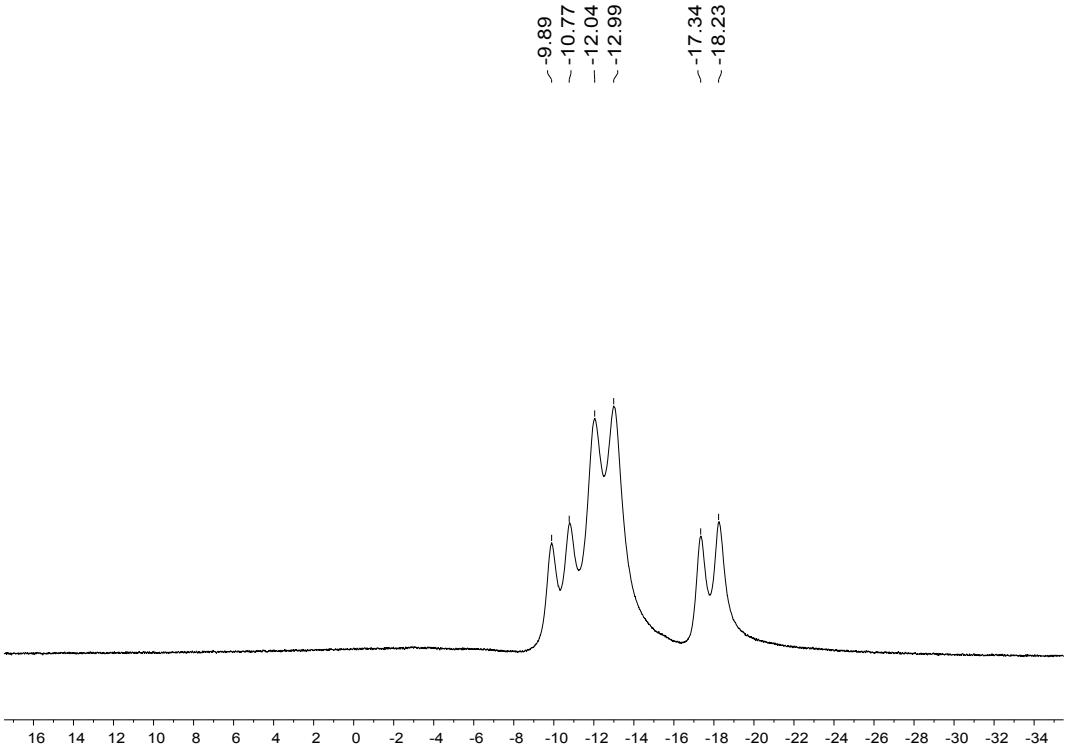

Fig. S24. ^{11}B NMR (Acetone-D_6, 160.46 MHz) spectrum of Compound **3d**.

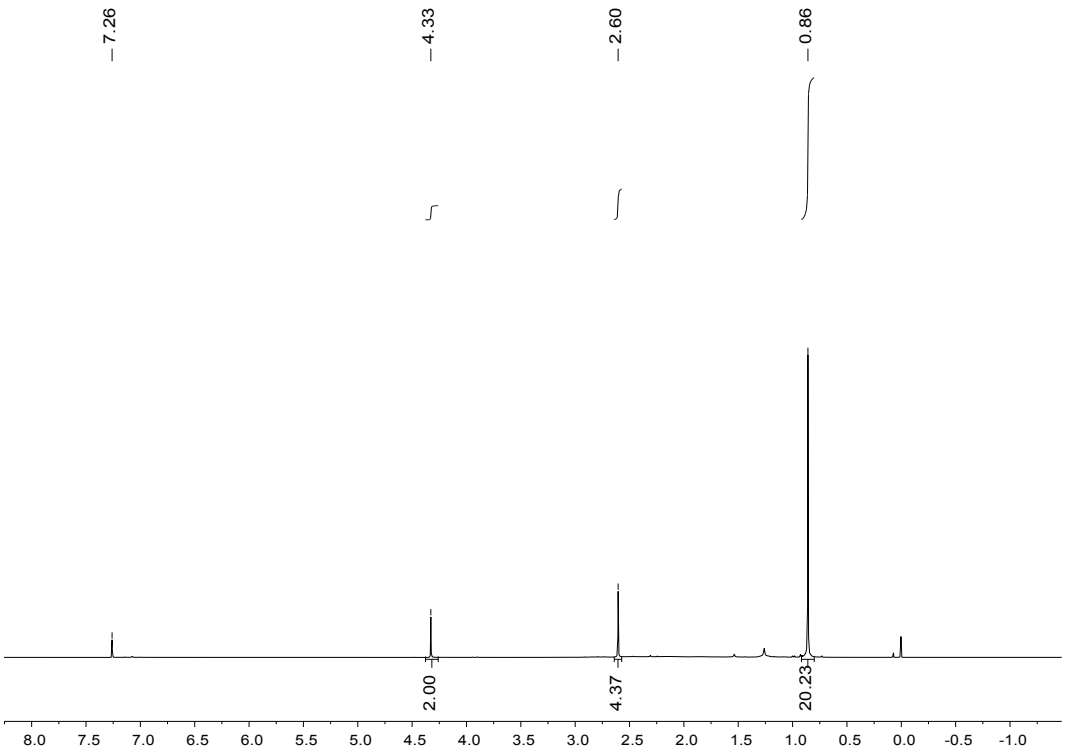

Fig. S25. ^{1}H NMR ($CDCl_3$, 500.13 MHz) spectrum of Compound **4a**.

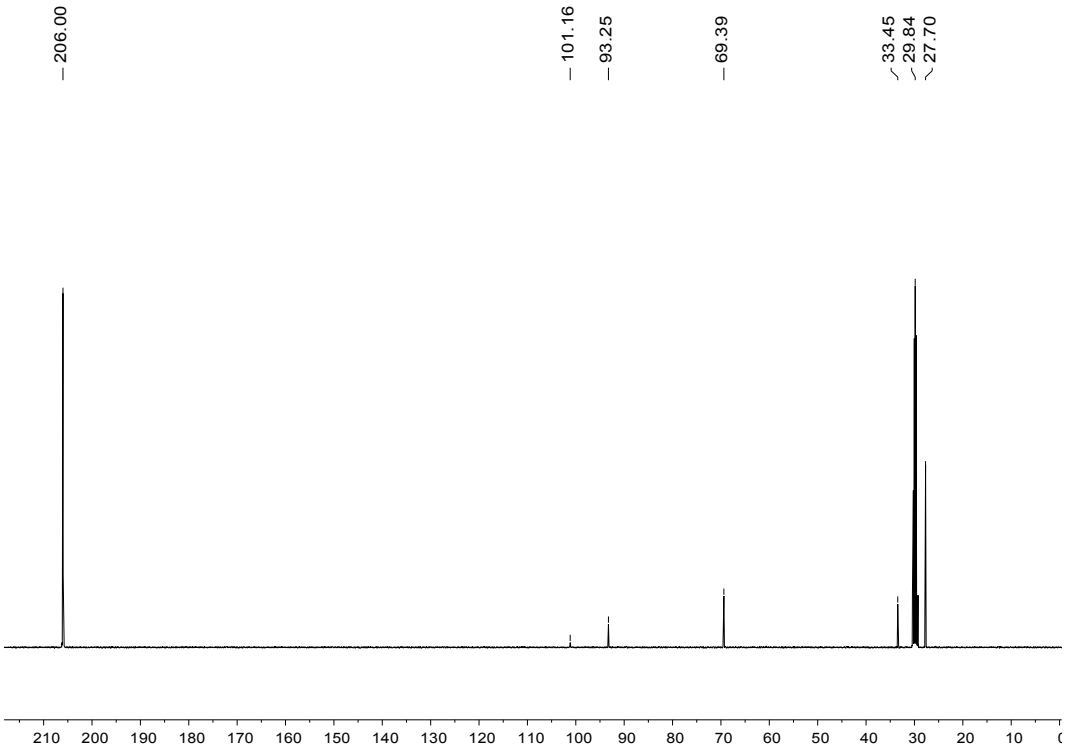

Fig. S26. $^{13}C\{^{1}H\}$ NMR (Acetone-D_6, 100.62 MHz) spectrum of Compound **4a**.

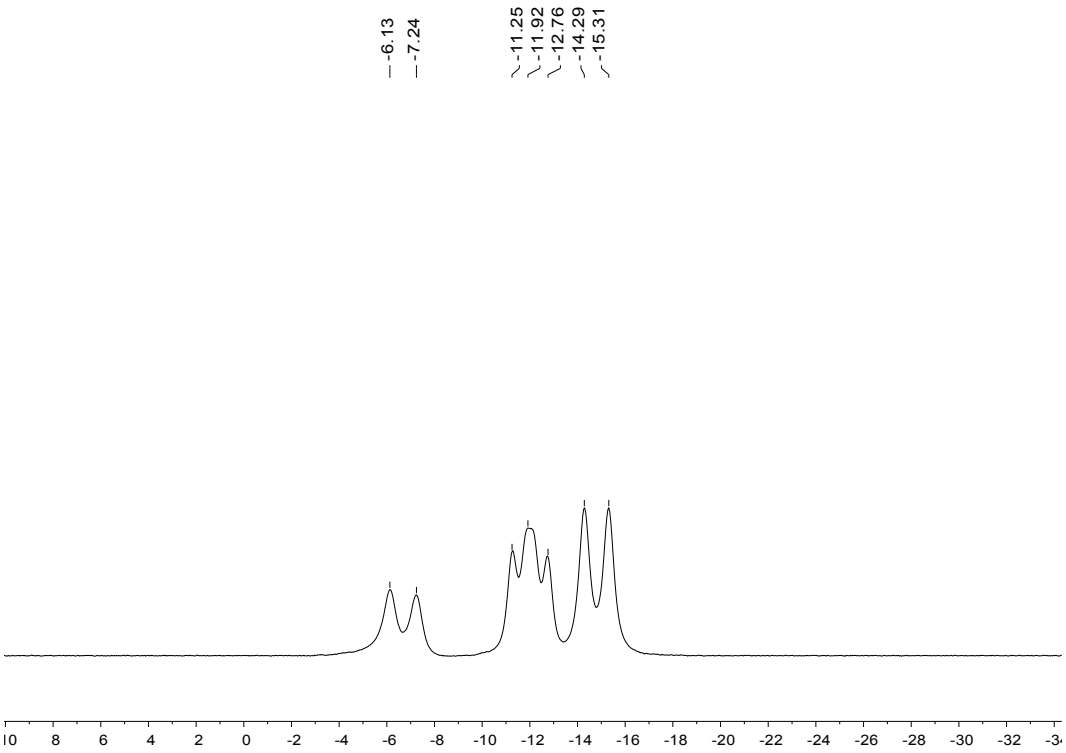

Fig. S27. ^{11}B NMR (Acetone-D_6, 160.46 MHz) spectrum of Compound **4a**.

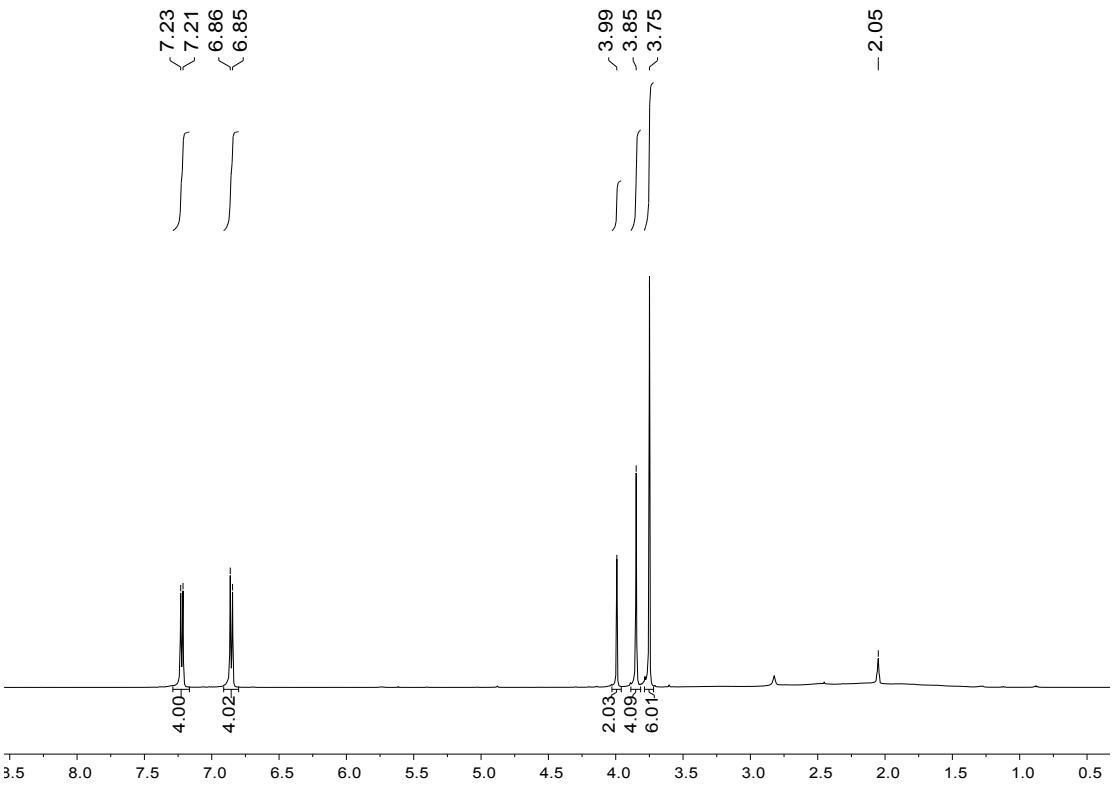

Fig. S28. ^{1}H NMR (Acetone-D_6, 400.13 MHz) spectrum of Compound **4d**.

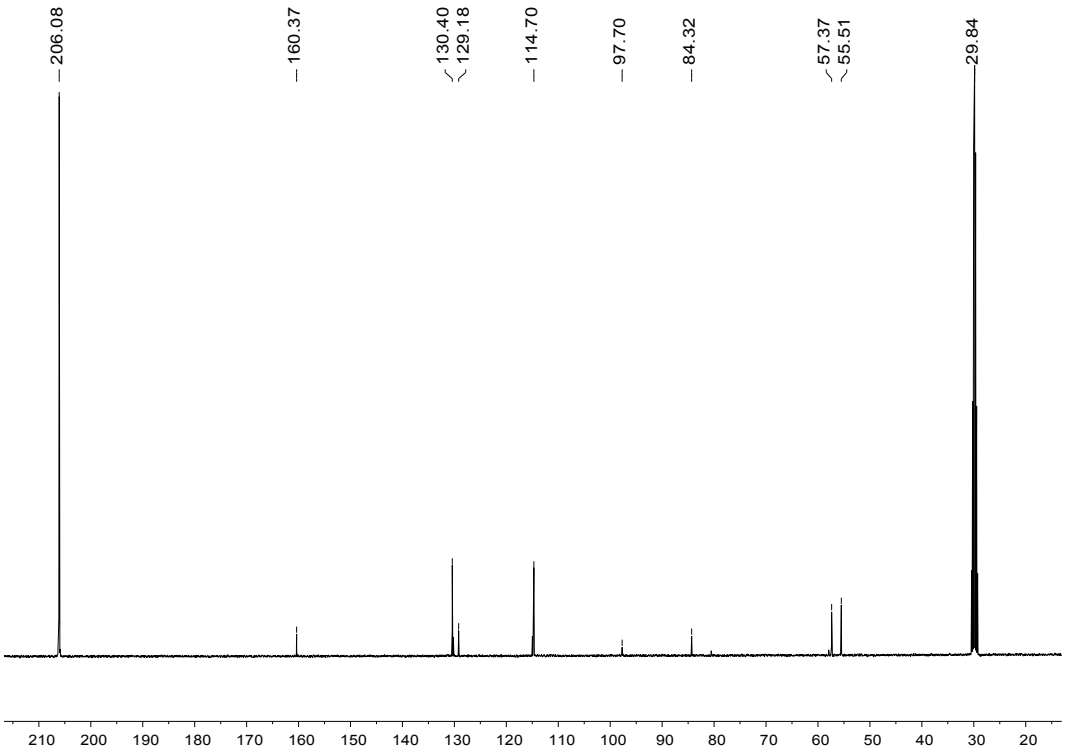

Fig. S29. $^{13}C\{^{1}H\}$ NMR (Acetone-D_6, 100.62 MHz) spectrum of Compound **4d**.

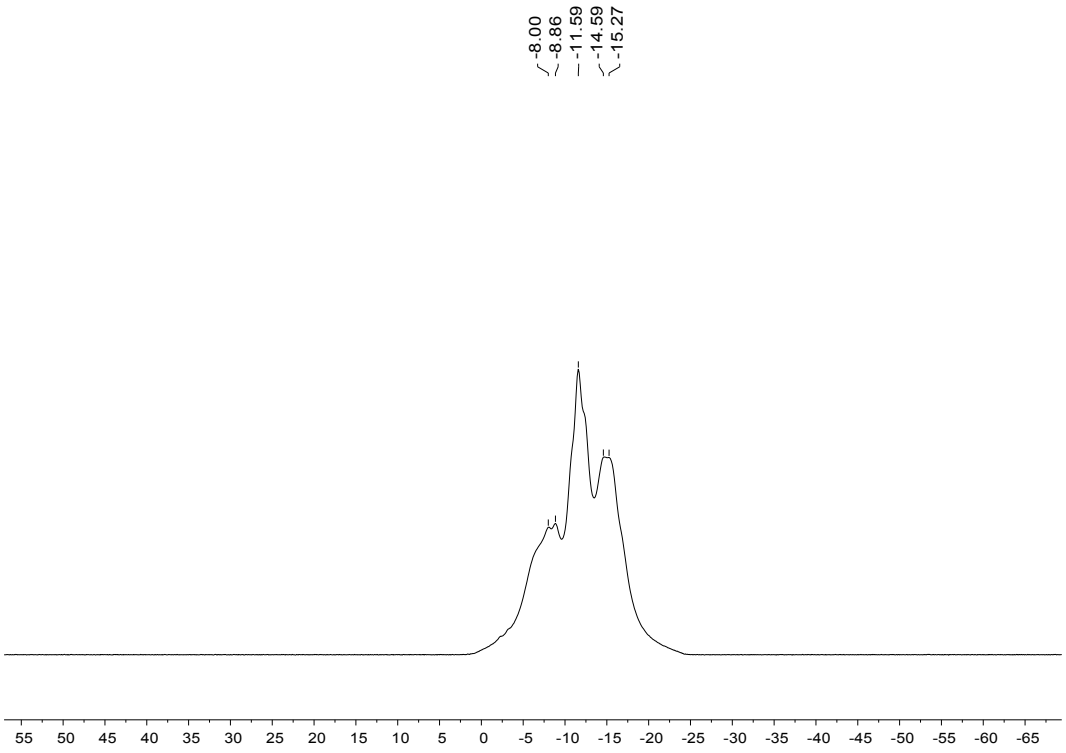

Fig. S30. ^{11}B NMR (Acetone-D_6, 160.46 MHz) spectrum of Compound **4d**.

(2) X-ray crystallography.

Molecular structures of **2b**, **2c**, **3a**, **3b**, **3d** and **4a**, as well as the pertinent structure parameters, were given in Fig. S31-S36. Crystal data, data collection parameters, and the results of the analysis of these compounds are listed in Tables S1. Two crystallographically independent molecules were found in the asymmetric units of **3a**, both of which were plotted in Fig. S33. In asymmetric units of **3a** and **4a**, there are disorders in *t*Bu groups. Therefore, PART, SIMU, DFIX and/or DELU instructions were used to refine the structures to convergence.

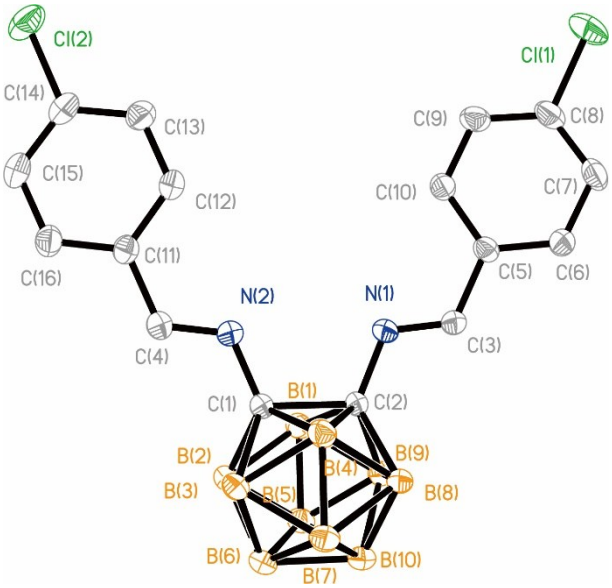

Fig. S31. Molecular structure of **2b** (Hydrogen atoms are omitted for clarity, ellipsoids set at the 30% probability level.) Selected bond lengths (pm) and angles(°): C(1)-C(2) 171.8(3), C(1)-N(2) 141.4(3), C(2)-N(1) 141.4(3), N(1)-C(3) 126.2(3), N(2)-C(4) 125.8(4); N(2)-C(1)-C(2) 112.7(2), N(1)-C(2)-C(1) 113.04(19), C(3)-N(1)-C(2) 118.8(2), C(4)-N(2)-C(1) 120.1(2), N(1)-C(3)-C(5) 121.4(2), N(2)-C(4)-C(11) 120.5(3).

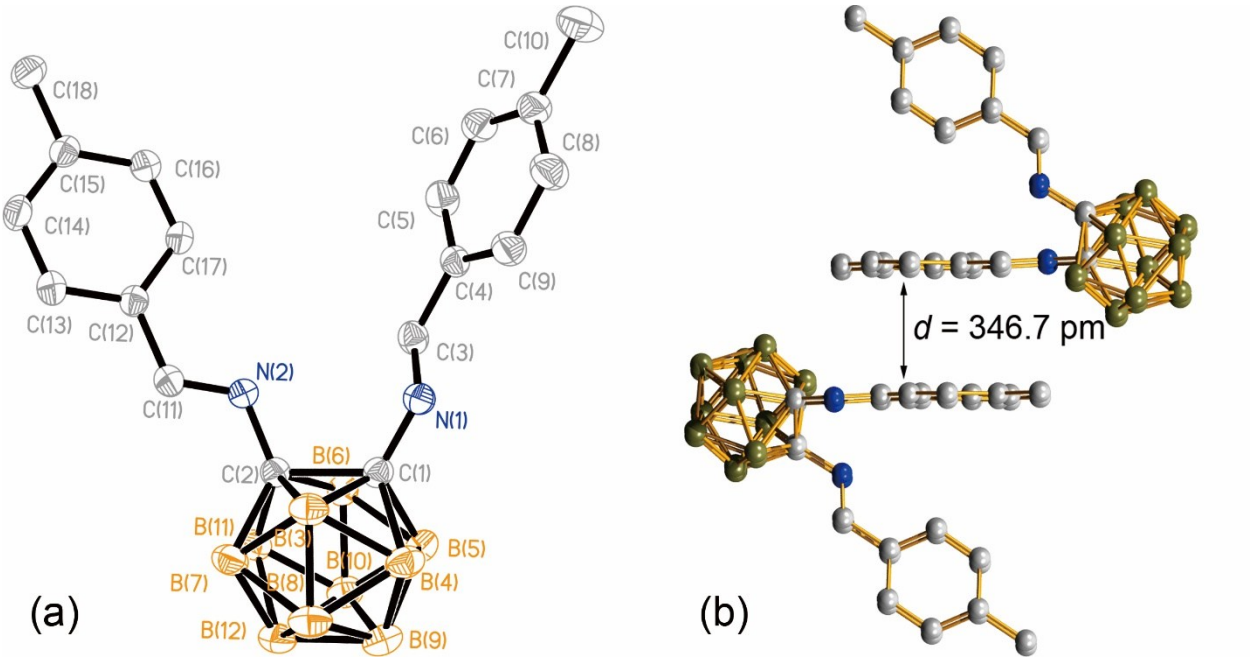

Fig. S32. Molecular structure of **2c** (Hydrogen atoms are omitted for clarity, ellipsoids set at the 30% probability level.) Selected bond lengths (pm) and angles(°): C(1)-C(2) 172.3(2), C(1)-N(1) 141.4(2), C(2)-N(2) 141.6(2), N(1)-C(3) 126.9(2), C(11)-N(2) 126.1(2); N(1)-C(1)-C(2) 120.69(13), N(2)-C(2)-C(1) 112.38(12), C(3)-N(1)-C(1) 121.45(15), C(11)-N(2)-C(2) 120.61(15), N(2)-C(11)-C(12) 122.25(16), N(1)-C(3)-C(4) 121.31(16).

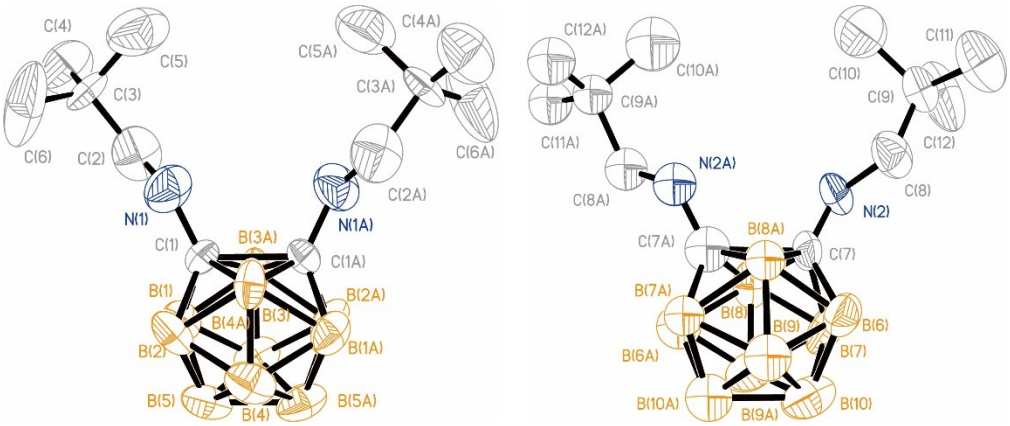

Fig. S33. Molecular structure of **3a** (Hydrogen atoms are omitted for clarity, ellipsoids set at the 30% probability level.) Selected bond lengths (pm) and angles(°): C(1)-C(1A) 188.2(13), C(7)-C(7A) 185.3(13), N(1)-C(2) 139.4(9), N(1)-C(1) 139.9(9), N(2)-C(8) 144.4(15); C(2)-N(1)-C(1) 123.4(8), N(1)-C(1)-C(1A) 115.5(4), N(2)-C(7)-C(7A) 118.2(5), C(7)-N(2)-C(8) 116.6(12).

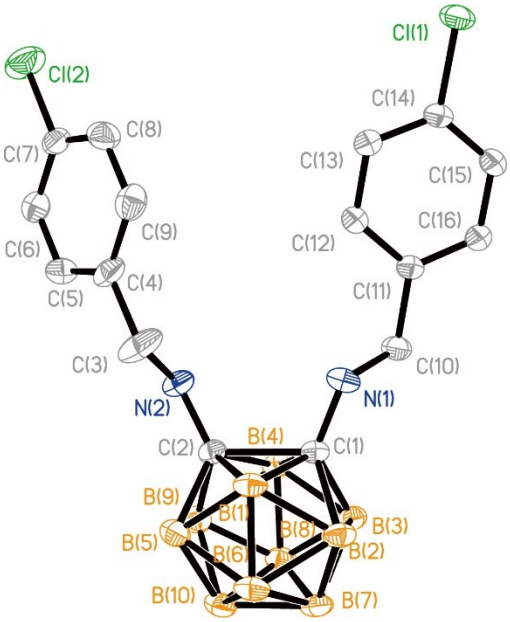

Fig. S34. Molecular structure of **3b** (Hydrogen atoms are omitted for clarity, ellipsoids set at the 30% probability level.) Selected bond lengths (pm) and angles(°): C(1)-C(2) 187.1(3), C(1)-N(1) 139.2(2), C(2)-N(2) 138.5(2), N(1)-C(10) 146.1(3), N(2)-C(3) 145.5(3); N(1)-C(1)-C(2) 113.19(15), N(2)-C(2)-C(1) 116.41(16), C(1)-N(1)-C(10) 120.70(17), C(2)-N(2)-C(3) 122.76(19).

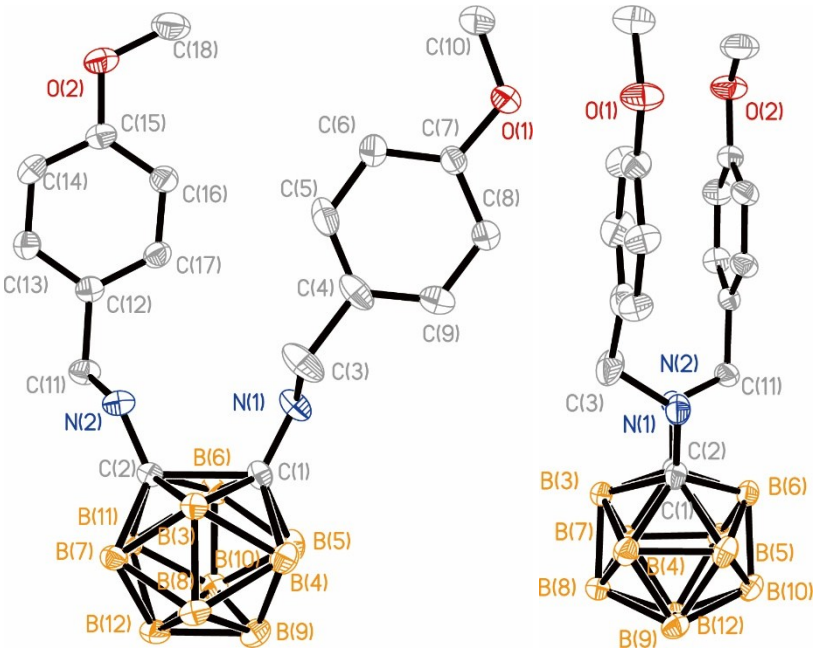

Fig. S35. Molecular structure of **3d** (Hydrogen atoms are omitted for clarity, ellipsoids set at the 30% probability level.) Selected bond lengths (pm) and angles(°): C(1)-C(2) 193.2(3), C(1)-N(1) 138.0(3), C(2)-N(2) 137.4(3), C(3)-N(1) 145.6(3), C(11)-N(2) 146.2(3); N(1)-C(1)-C(2) 116.85(17), N(2)-C(2)-C(1) 113.81(15), C(1)-N(1)-C(3) 121.26(19), C(2)-N(2)-C(11) 122.59(18).

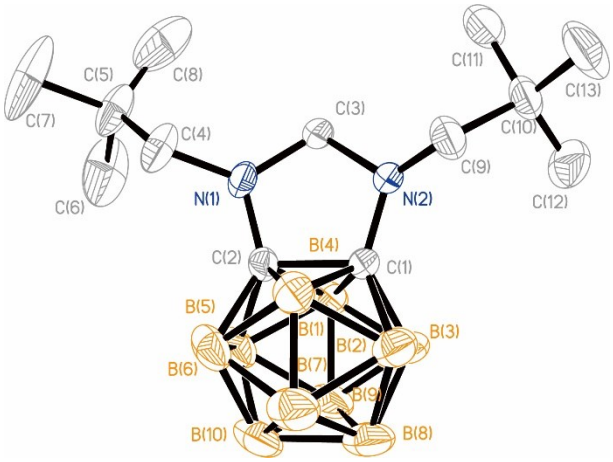

Fig. S36. Molecular structure of **4a** (Hydrogen atoms are omitted for clarity, ellipsoids set at the 30% probability level.) Selected bond lengths (pm) and angles(°): C(2)-C(1) 162.4(3), N(2)-C(1) 140.5(3), N(2)-C(3) 160.1(10), C(2)-N(1) 141.4(3), N(1)-C(3) 148.7(10); C(9)-N(2)-C(1) 124.2(3), C(9)-N(2)-C(3) 126.1(5), C(1)-N(2)-C(3) 106.3(3), N(1)-C(2)-C(1) 104.81(17), N(2)-C(1)-C(2) 105.95(18), C(2)-N(1)-C(4) 119.1(2), C(2)-N(1)-C(3) 109.9(3), C(4)-N(1)-C(3) 128.8(5), N(1)-C(3)-N(2) 100.3(7).

Table S1. Details of crystallographic data for **2b**, **2c**, **3a**, **3b**, **3d** and **4a.**

	2b	**2c**	**3a**	**3b**	**3d**	**4a**
CCDC Nos.	1881761	1881762	1881763	1881764	1881765	1881766
Empirical formula	$C_{16}H_{20}B_{10}Cl_2N_2$	$C_{18}H_{26}B_{10}N_2$	$C_{12}H_{34}B_{10}N_2$	$C_{16}H_{24}B_{10}Cl_2N_2$	$C_{18}H_{30}B_{10}N_2O_2$	$C_{13}H_{34}B_{10}N_2$
Formula weight	419.34	378.51	314.51	423.37	414.54	326.52
Temperature (K)	296(2)	296(2)	296(2)	296(2)	296(2)	296(2)
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Monoclinic	Orthorhombic	Triclinic	Orthorhombic	Triclinic
space group	P_{-1}	*P*2(1)/c	*F*dd2	P_{-1}	*P*na2(1)	P_{-1}
a (Å)	7.133(2)	7.4532(17)	11.268(8)	7.3966(11)	26.797(6)	8.829(5)
b (Å)	12.872(4)	13.427(3)	19.419(14)	11.6224(18)	7.6904(17)	11.088(5)
c (Å)	13.741(4)	22.271(5)	39.46(3)	13.104(2)	11.398(3)	12.660(6)
α (°)	66.302(4)	90	90	85.700(2)	90	107.034(9)
β (°)	75.196(5)	92.261(6)	90	82.407(2)	90	98.560(9)
γ (°)	83.836(5)	90	90	85.925(2)	90	109.841(6)
V (Å ^{3})	1117.0(5)	2227.1(9)	8635(11)	1111.3(3)	2348.8(9)	1071.4(10)
Z	2	4	16	2	4	2
D_{calcd} (Mg / m^3)	1.247	1.129	0.968	1.265	1.172	1.012
μ (mm^{-1})	0.297	0.059	0.049	0.299	0.067	0.052
F(000)	428	792	2720	436	872	352
θ range (°)	1.664 to 25.493	1.771 to 27.543	2.06 to 27.52	1.571 to 27.503	1.520 to 28.108	1.75 to 25.09

Limiting indices	-8<=h<=8, -15<=k<=15, -16<=l<=16	-6<=h<=9, -17<=k<=17, -28<=l<=28	-12<=h<=14, -24<=k<=24, -50<=l<=51	-9<=h<=9, -15<=k<=14, -13<=l<=16	-29<=h<=34, -9<=k<=9, -14<=l<=14	-10<=h<=10, -9<=k<=13, -15<=l<=15
Ref. collected/unique	7071 / 4112	14217 / 5087	15542 / 4916	8385 / 5046	15891 / 5315	6571 / 3725
R_{int}	0.0283	0.0359	0.1175	0.0185	0.0273	0.0389
Completeness to θ [%]	98.6	99.5	99.8	99.1	99.2	97.7
Data / restraints / parameters	4112 / 0 / 351	5087 / 0 / 313	4916 / 56 / 242	5046 / 0 / 319	5315 / 3 / 340	3725 / 16 / 318
GOOF [a]	1.003	1.013	1.121	1.035	1.035	1.001
Final R indices [I > 2σ(I)] [b]	R_1 = 0.0618, wR_2 = 0.1943	R_1 = 0.0496, wR_2 = 0.1219	R_1 = 0.0960, wR_2 = 0.1791	R_1 = 0.0555, wR_2 = 0.1610	R_1 = 0.0395, wR_2 = 0.1052	R_1 = 0.0754, wR_2 = 0.2098
R indices (all data)	R_1 = 0.0791, wR_2 = 0.2156	R_1 = 0.0962, wR_2 = 0.1470	R_1 = 0.2832, wR_2 = 0.2295	R_1 = 0.0664, wR_2 = 0.1736	R_1 = 0.0460, wR_2 = 0.1109	R_1 = 0.1288, wR_2 = 0.2463
$\Delta\rho_{max, min}$ (e/Å^3)	0.393 and -0.428	0.144 and -0.149	0.184 and -0.117	1.071 and -0.770	0.277 and -0.208	0.206 and -0.162

[a] Goodness-of-fit on F^2 [b] $R_1 = ||Fo|-|Fc||/|Fo|$, $wR_2 = [\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$

(3) Computational details

All quantum chemical calculations were carried out using the Gaussian09/Gaussian16 package.[1] The molecular structure optimizations were performed using the B3LYP, B3LYP-D3, B3PW91 or B3PW91-D3 functional along with the cc-pVTZ basis set.[2] Every stationary point was identified by a subsequent frequency calculation either as minimum (Number of imaginary frequencies NIMAG: 0) or transition state (NIMAG: 1).

Table S2. SCF energies, E(SCF), and free Gibbs enthalpies, G^{298}, for calculated compounds.

Compound	Functionals	E(SCF) [a.u.]	NIMAG, $\tilde{\nu}$ [cm^{-1}]	G^{298} [a.u.]
2c	B3PW91-D3	-1059.736150	0	-1059.358841
2c'	B3PW91-D3	-1059.735843	0	-1059.360276
TS1	B3PW91-D3	-1059.734026	1, -48.7	-1059.355783
2b	B3LYP	-1900.664431	0	-1900.360226
2b	B3LYP-D3	-1900.726192	0	-1900.421351
2b	B3PW91	-1900.189432	0	-1899.884279
2b	B3PW91-D3	-1900.258326	0	-1899.952647
3b	B3LYP	-1903.098634	0	-1902.750006
3b	B3LYP-D3	-1903.169470	0	-1902.818507
3b	B3PW91	-1902.629611	0	-1902.279805
3b	B3PW91-D3	-1902.709776	0	-1902.357177

Compound **2c** at B3PW91-D3/cc-pVTZ level.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.216053	-1.102214	-0.058754
2	6	0	2.118642	0.627200	-0.029284
3	7	0	1.056869	-1.868569	-0.214499
4	5	0	3.387096	1.274053	0.902591
5	5	0	2.647547	-0.194670	-1.454029
6	5	0	3.429040	1.292563	-0.871349
7	5	0	3.609827	-1.573239	-0.910186
8	5	0	4.321438	-0.118122	1.463524
9	5	0	2.568786	-0.219065	1.392313
10	5	0	4.408164	-0.075616	-1.418488
11	5	0	3.544952	-1.601798	0.863018

12	5	0	4.869799	0.822617	0.050259
13	5	0	4.972984	-0.951358	0.027025
14	6	0	-1.215983	-2.401281	0.298050
15	6	0	0.556578	2.342056	-0.028599
16	1	0	1.356045	3.086309	0.043942
17	6	0	0.018349	-1.653542	0.491030
18	1	0	-0.009939	-0.891136	1.270611
19	6	0	-1.907878	1.993224	-0.186952
20	1	0	-1.738078	0.927295	-0.269847
21	6	0	-0.807636	2.849965	-0.064662
22	6	0	-3.418528	3.883667	-0.109680
23	6	0	-2.320531	4.729921	0.009932
24	1	0	-2.476388	5.799494	0.087206
25	6	0	-2.325042	-2.088167	1.082227
26	1	0	-2.248000	-1.303775	1.827265
27	6	0	-1.030621	4.221945	0.031182
28	1	0	-0.186574	4.896132	0.125753
29	6	0	-3.187192	2.506543	-0.207868
30	1	0	-4.031303	1.832943	-0.304604
31	6	0	-1.331274	-3.410706	-0.663457
32	1	0	-0.471073	-3.647953	-1.276033
33	6	0	-3.522381	-2.766482	0.914327
34	1	0	-4.375510	-2.510333	1.531686
35	6	0	-3.642027	-3.774948	-0.037213
36	6	0	-2.524728	-4.083218	-0.821855
37	1	0	-2.603143	-4.864559	-1.569496
38	6	0	-4.818124	4.419571	-0.144852
39	1	0	-5.283600	4.224078	-1.114339
40	1	0	-4.843306	5.495067	0.028569
41	1	0	-5.441130	3.938296	0.612410
42	6	0	-4.926018	-4.526696	-0.221466
43	1	0	-4.806407	-5.573803	0.068747
44	1	0	-5.239061	-4.518425	-1.267842
45	1	0	-5.731696	-4.103225	0.377904
46	7	0	0.806968	1.096614	-0.073383
47	1	0	1.781281	-0.260931	2.270819
48	1	0	3.145014	2.258567	1.515382
49	1	0	3.211859	2.291673	-1.469735
50	1	0	5.822081	1.528049	0.088680
51	1	0	3.526591	-2.577578	-1.527238
52	1	0	3.432131	-2.621426	1.451264
53	1	0	5.015901	-0.021854	-2.434759
54	1	0	4.866613	-0.102720	2.516131
55	1	0	6.005254	-1.533721	0.052078

56	1	0	1.887480	-0.220626	-2.355407

Compound **2c'** at B3PW91-D3/cc-pVTZ level.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.854588	1.886494	0.000062
2	6	0	0.854594	1.886492	-0.000045
3	7	0	-1.424709	0.613346	0.000034
4	5	0	1.433224	3.220097	-0.885493
5	5	0	0.000090	2.325630	1.427541
6	5	0	1.433333	3.220023	0.885438
7	5	0	-1.433216	3.220028	0.885616
8	5	0	-0.000084	4.092095	-1.443557
9	5	0	-0.000083	2.325745	-1.427488
10	5	0	0.000094	4.091978	1.443751
11	5	0	-1.433323	3.220098	-0.885314
12	5	0	0.888725	4.651602	0.000065
13	5	0	-0.888713	4.651604	0.000174
14	6	0	-3.334916	-0.819365	0.000060
15	6	0	2.689998	0.486698	-0.000233
16	1	0	3.358106	1.354327	-0.000329
17	6	0	-2.689995	0.486703	0.000113
18	1	0	-3.358101	1.354333	0.000216
19	6	0	2.593473	-2.005891	-0.000061
20	1	0	1.512961	-1.942986	-0.000013
21	6	0	3.334917	-0.819372	-0.000217
22	6	0	4.634255	-3.308863	-0.000268
23	6	0	5.365638	-2.125352	-0.000557
24	1	0	6.448536	-2.166524	-0.000897
25	6	0	-4.726061	-0.895093	0.000186
26	1	0	-5.311775	0.017587	0.000335
27	6	0	4.726060	-0.895102	-0.000499
28	1	0	5.311776	0.017576	-0.000795
29	6	0	3.236980	-3.225212	-0.000120
30	1	0	2.653014	-4.138905	-0.000141
31	6	0	-2.593476	-2.005885	-0.000098
32	1	0	-1.512965	-1.942983	-0.000170
33	6	0	-5.365642	-2.125339	0.000146
34	1	0	-6.448540	-2.166509	0.000265
35	6	0	-4.634260	-3.308854	-0.000032

36	6	0	-3.236987	-3.225206	-0.000137
37	1	0	-2.653023	-4.138900	-0.000239
38	6	0	5.311365	-4.646553	0.000991
39	1	0	5.033697	-5.222984	0.886905
40	1	0	6.396700	-4.549740	-0.011462
41	1	0	5.014125	-5.235162	-0.870315
42	6	0	-5.311388	-4.646536	-0.000293
43	1	0	-5.022297	-5.230120	0.877167
44	1	0	-5.025516	-5.228048	-0.880203
45	1	0	-6.396787	-4.549662	0.001761
46	7	0	1.424712	0.613343	-0.000105
47	1	0	-0.000139	1.540971	-2.307605
48	1	0	2.437885	3.053243	-1.489685
49	1	0	2.438069	3.053112	1.489490
50	1	0	1.533224	5.646775	0.000066
51	1	0	-2.437878	3.053124	1.489793
52	1	0	-2.438060	3.053239	-1.489381
53	1	0	0.000159	4.668282	2.479605
54	1	0	-0.000148	4.668481	-2.479364
55	1	0	-1.533211	5.646778	0.000253
56	1	0	0.000145	1.540785	2.307594

TS1 at B3PW91-D3/cc-pVTZ level.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.997606	-1.228353	-0.169891
2	6	0	2.116239	0.464663	-0.040741
3	7	0	0.731916	-1.780411	-0.428848
4	5	0	3.430488	0.893602	0.964795
5	5	0	2.599051	-0.312605	-1.500762
6	5	0	3.541706	1.012201	-0.800452
7	5	0	3.336978	-1.840077	-1.009434
8	5	0	4.163337	-0.635317	1.469337
9	5	0	2.416894	-0.502567	1.349421
10	5	0	4.352911	-0.437738	-1.402602
11	5	0	3.217834	-1.962581	0.761297
12	5	0	4.873588	0.303569	0.130206
13	5	0	4.741862	-1.467198	0.001700
14	6	0	-1.401337	-2.576877	0.289610
15	6	0	0.801856	2.367355	0.003944

16	1	0	1.699321	2.991059	0.068435
17	6	0	-0.076152	-2.022385	0.523184
18	1	0	0.182223	-1.824729	1.567428
19	6	0	-1.689592	2.382042	-0.110277
20	1	0	-1.675391	1.302416	-0.188013
21	6	0	-0.474347	3.068456	-0.006966
22	6	0	-2.905103	4.474190	-0.019347
23	6	0	-1.693450	5.150479	0.082417
24	1	0	-1.689609	6.231507	0.157811
25	6	0	-2.235161	-2.829817	1.377538
26	1	0	-1.884343	-2.616628	2.381294
27	6	0	-0.492024	4.458419	0.087882
28	1	0	0.443247	5.001478	0.167532
29	6	0	-2.879733	3.077923	-0.115706
30	1	0	-3.815407	2.536070	-0.197115
31	6	0	-1.869521	-2.852337	-0.999816
32	1	0	-1.221929	-2.650599	-1.843176
33	6	0	-3.506170	-3.348695	1.186494
34	1	0	-4.142141	-3.539468	2.042963
35	6	0	-3.976478	-3.628036	-0.093278
36	6	0	-3.135157	-3.368660	-1.181365
37	1	0	-3.488626	-3.577857	-2.184806
38	6	0	-4.211943	5.208824	-0.031619
39	1	0	-4.745778	5.037039	-0.969642
40	1	0	-4.072431	6.283314	0.084354
41	1	0	-4.862392	4.862368	0.775007
42	6	0	-5.342113	-4.205897	-0.313647
43	1	0	-5.271677	-5.240146	-0.661155
44	1	0	-5.887138	-3.647837	-1.077843
45	1	0	-5.935245	-4.200783	0.600600
46	7	0	0.872468	1.099026	-0.056554
47	1	0	1.602292	-0.463801	2.201937
48	1	0	3.287375	1.865877	1.626168
49	1	0	3.482419	2.066558	-1.336974
50	1	0	5.908200	0.872213	0.240675
51	1	0	3.144355	-2.789599	-1.686745
52	1	0	2.944347	-2.995590	1.270121
53	1	0	5.000312	-0.412685	-2.395190
54	1	0	4.671542	-0.746379	2.534703
55	1	0	5.685779	-2.184434	0.012469
56	1	0	1.872241	-0.193889	-2.421054

Compound **2b** at **B3LYP**/cc-pVTZ level.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.867727	2.253835	0.000082
2	6	0	0.867727	2.253835	-0.000017
3	7	0	-1.446658	0.978348	0.000069
4	5	0	1.435765	3.591405	-0.886677
5	5	0	0.000079	2.692190	1.427611
6	5	0	1.435864	3.591345	0.886669
7	5	0	-1.435765	3.591346	0.886831
8	5	0	-0.000081	4.458683	-1.444136
9	5	0	-0.000080	2.692286	-1.427517
10	5	0	0.000081	4.458586	1.444348
11	5	0	-1.435864	3.591404	-0.886515
12	5	0	0.887892	5.021486	0.000075
13	5	0	-0.887892	5.021486	0.000175
14	6	0	-3.363839	-0.462476	0.000119
15	6	0	2.712417	0.846508	-0.000167
16	1	0	3.383634	1.708887	-0.000158
17	6	0	-2.712417	0.846508	0.000142
18	1	0	-3.383634	1.708887	0.000213
19	6	0	2.629236	-1.654228	-0.000128
20	1	0	1.550181	-1.601323	-0.000091
21	6	0	3.363839	-0.462476	-0.000170
22	6	0	4.665645	-2.915506	-0.000186
23	6	0	5.417117	-1.748787	-0.000226
24	1	0	6.495753	-1.798794	-0.000264
25	6	0	-4.759262	-0.527406	0.000203
26	1	0	-5.337886	0.387592	0.000284
27	6	0	4.759262	-0.527405	-0.000216
28	1	0	5.337886	0.387592	-0.000247
29	6	0	3.273074	-2.877566	-0.000136
30	1	0	2.711303	-3.800036	-0.000105
31	6	0	-2.629236	-1.654228	0.000015
32	1	0	-1.550181	-1.601323	-0.000051
33	6	0	-5.417117	-1.748787	0.000186
34	1	0	-6.495753	-1.798794	0.000252
35	6	0	-4.665645	-2.915506	0.000083
36	6	0	-3.273074	-2.877567	-0.000004
37	1	0	-2.711303	-3.800036	-0.000084
38	7	0	1.446657	0.978348	-0.000088

39	1	0	-0.000129	1.919234	-2.312052
40	1	0	2.435102	3.434733	-1.492976
41	1	0	2.435269	3.434631	1.492846
42	1	0	1.528843	6.013178	0.000073
43	1	0	-2.435102	3.434634	1.493119
44	1	0	-2.435269	3.434731	-1.492702
45	1	0	0.000139	5.033509	2.475460
46	1	0	-0.000139	5.033674	-2.475209
47	1	0	-1.528843	6.013178	0.000243
48	1	0	0.000129	1.919079	2.312094
49	17	0	5.478723	-4.461285	-0.000196
50	17	0	-5.478723	-4.461285	0.000059

Compound **2b** at **B3LYP-D3**/cc-pVTZ level.

23	6	0	5.356016	-1.785321	-0.000252
24	1	0	6.433290	-1.858011	-0.000297
25	6	0	-4.722607	-0.551011	0.000182
26	1	0	-5.319473	0.352211	0.000234
27	6	0	4.722607	-0.551011	-0.000206
28	1	0	5.319473	0.352211	-0.000215
29	6	0	3.189283	-2.872103	-0.000182
30	1	0	2.610457	-3.783887	-0.000173
31	6	0	-2.569950	-1.636587	0.000053
32	1	0	-1.492004	-1.561525	0.000006
33	6	0	-5.356016	-1.785321	0.000176
34	1	0	-6.433290	-1.858011	0.000222
35	6	0	-4.581345	-2.937110	0.000108
36	6	0	-3.189283	-2.872103	0.000046
37	1	0	-2.610457	-3.783887	-0.000006
38	7	0	1.434227	0.999442	-0.000042
39	1	0	-0.000100	1.934766	-2.309288
40	1	0	2.438666	3.449890	-1.490474
41	1	0	2.438794	3.449814	1.490421
42	1	0	1.529699	6.037164	0.000078
43	1	0	-2.438666	3.449815	1.490632
44	1	0	-2.438794	3.449889	-1.490263
45	1	0	0.000108	5.058513	2.478038
46	1	0	-0.000108	5.058638	-2.477799
47	1	0	-1.529699	6.037164	0.000210
48	1	0	0.000100	1.934649	2.309370
49	17	0	5.364029	-4.498992	-0.000297
50	17	0	-5.364029	-4.498992	0.000099

Compound **2b** at **B3PW91**/cc-pVTZ level.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.856157	2.221905	0.000080
2	6	0	0.856157	2.221905	-0.000028
3	7	0	-1.437737	0.950522	0.000066
4	5	0	1.431820	3.556127	-0.884366
5	5	0	0.000088	2.661462	1.426980
6	5	0	1.431929	3.556061	0.884337
7	5	0	-1.431820	3.556063	0.884516
8	5	0	-0.000090	4.427312	-1.441459
9	5	0	-0.000088	2.661566	-1.426895
10	5	0	0.000090	4.427207	1.441673
11	5	0	-1.431929	3.556126	-0.884188
12	5	0	0.887322	4.986810	0.000072
13	5	0	-0.887323	4.986810	0.000182
14	6	0	-3.372395	-0.457968	0.000118
15	6	0	2.704706	0.838995	-0.000197
16	1	0	3.362442	1.713777	-0.000188
17	6	0	-2.704706	0.838995	0.000150
18	1	0	-3.362442	1.713777	0.000229
19	6	0	2.653838	-1.656661	-0.000114
20	1	0	1.572690	-1.615704	-0.000074
21	6	0	3.372395	-0.457968	-0.000179
22	6	0	4.704128	-2.889483	-0.000159
23	6	0	5.439496	-1.713854	-0.000222
24	1	0	6.520100	-1.750866	-0.000263
25	6	0	-4.766530	-0.503263	0.000213
26	1	0	-5.332710	0.421223	0.000309
27	6	0	4.766530	-0.503263	-0.000229
28	1	0	5.332710	0.421223	-0.000277
29	6	0	3.312561	-2.869795	-0.000104
30	1	0	2.763111	-3.801346	-0.000056
31	6	0	-2.653838	-1.656661	-0.000005
32	1	0	-1.572690	-1.615704	-0.000080
33	6	0	-5.439496	-1.713854	0.000189
34	1	0	-6.520100	-1.750866	0.000264
35	6	0	-4.704128	-2.889483	0.000066
36	6	0	-3.312561	-2.869795	-0.000032
37	1	0	-2.763111	-3.801346	-0.000127

38	7	0	1.437737	0.950522	-0.000103
39	1	0	-0.000143	1.881995	-2.310950
40	1	0	2.434674	3.392855	-1.490930
41	1	0	2.434859	3.392743	1.490764
42	1	0	1.532413	5.980238	0.000068
43	1	0	-2.434674	3.392746	1.491067
44	1	0	-2.434858	3.392852	-1.490627
45	1	0	0.000154	5.001229	2.477522
46	1	0	-0.000154	5.001410	-2.477267
47	1	0	-1.532413	5.980238	0.000257
48	1	0	0.000143	1.881827	2.310977
49	17	0	5.531590	-4.413407	-0.000146
50	17	0	-5.531590	-4.413407	0.000034

Compound **2b** at **B3PW91-D3**/cc-pVTZ level.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.854056	2.253559	0.000089
2	6	0	0.854057	2.253559	0.000041
3	7	0	-1.424591	0.979850	0.000074
4	5	0	1.433470	3.586302	-0.885459
5	5	0	0.000038	2.691688	1.428106
6	5	0	1.433518	3.586266	0.885561
7	5	0	-1.433470	3.586269	0.885640
8	5	0	-0.000039	4.457998	-1.443906
9	5	0	-0.000037	2.691742	-1.427959
10	5	0	0.000039	4.457943	1.444121
11	5	0	-1.433517	3.586300	-0.885380
12	5	0	0.888695	5.017733	0.000094
13	5	0	-0.888695	5.017733	0.000142
14	6	0	-3.330192	-0.455480	0.000112
15	6	0	2.689199	0.853984	-0.000045
16	1	0	3.358671	1.720116	-0.000122
17	6	0	-2.689199	0.853984	0.000115
18	1	0	-3.358670	1.720116	0.000175
19	6	0	2.580785	-1.635705	-0.000055
20	1	0	1.500884	-1.566586	0.000058
21	6	0	3.330192	-0.455480	-0.000126
22	6	0	4.599640	-2.919153	-0.000251
23	6	0	5.364494	-1.762214	-0.000332

24	1	0	6.443616	-1.827115	-0.000440
25	6	0	-4.722291	-0.534865	0.000187
26	1	0	-5.312265	0.374606	0.000248
27	6	0	4.722291	-0.534866	-0.000268
28	1	0	5.312265	0.374606	-0.000325
29	6	0	3.208311	-2.864650	-0.000118
30	1	0	2.636459	-3.782431	-0.000059
31	6	0	-2.580785	-1.635705	0.000033
32	1	0	-1.500884	-1.566586	-0.000027
33	6	0	-5.364494	-1.762213	0.000183
34	1	0	-6.443616	-1.827115	0.000241
35	6	0	-4.599640	-2.919152	0.000103
36	6	0	-3.208311	-2.864650	0.000028
37	1	0	-2.636459	-3.782431	-0.000034
38	7	0	1.424591	0.979850	0.000018
39	1	0	-0.000062	1.906174	-2.307347
40	1	0	2.437937	3.418121	-1.489489
41	1	0	2.438018	3.418056	1.489529
42	1	0	1.533283	6.012498	0.000096
43	1	0	-2.437938	3.418062	1.489662
44	1	0	-2.438017	3.418114	-1.489355
45	1	0	0.000068	5.033490	2.480071
46	1	0	-0.000068	5.033584	-2.479835
47	1	0	-1.533283	6.012498	0.000177
48	1	0	0.000062	1.906085	2.307464
49	17	0	5.388460	-4.463452	-0.000355
50	17	0	-5.388461	-4.463451	0.000102

Compound **3b** at **B3LYP**/cc-pVTZ level.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.571536	-2.201455	0.131377
2	6	0	-0.392529	-2.422635	-0.078569
3	5	0	0.715878	-2.642608	-1.334128
4	5	0	2.256662	-3.404243	-0.776987
5	5	0	2.150084	-3.530368	0.990654
6	5	0	0.579051	-2.756725	1.368157
7	5	0	-0.627495	-3.790699	-1.034204
8	5	0	0.960620	-4.394432	-1.481967
9	5	0	1.795994	-4.945473	0.000475

10	5	0	0.747991	-4.517801	1.388068
11	5	0	-0.751124	-3.807847	0.743212
12	5	0	0.052585	-5.144831	-0.134897
13	1	0	0.702074	-1.848417	-2.207874
14	1	0	3.256444	-3.155316	-1.350576
15	1	0	3.069554	-3.318446	1.700430
16	1	0	0.421411	-2.048668	2.298370
17	1	0	-1.573757	-3.757200	-1.736227
18	1	0	1.125631	-4.912117	-2.530349
19	1	0	2.537946	-5.864436	0.001239
20	1	0	0.712449	-5.131891	2.396068
21	1	0	-1.777674	-3.844174	1.324093
22	1	0	-0.457686	-6.207681	-0.204369
23	7	0	1.990327	-0.880776	0.230906
24	7	0	-1.157924	-1.284889	-0.122230
25	1	0	2.121387	-0.580900	1.185959
26	1	0	-0.994459	-0.678818	-0.909612
27	6	0	3.002467	-0.335996	-0.684061
28	6	0	-1.760944	-0.650919	1.047549
29	1	0	2.667881	-0.527792	-1.703375
30	1	0	3.965145	-0.841263	-0.561692
31	1	0	-1.030677	-0.064102	1.611519
32	1	0	-2.112113	-1.444914	1.707044
33	6	0	3.175954	1.145425	-0.458725
34	6	0	2.162939	2.043986	-0.797967
35	6	0	2.314457	3.406850	-0.591850
36	6	0	3.496767	3.880396	-0.035016
37	6	0	4.519421	3.011470	0.311688
38	6	0	4.349710	1.647791	0.096909
39	1	0	1.243493	1.674292	-1.232617
40	1	0	1.530479	4.098645	-0.863034
41	1	0	5.433471	3.393838	0.741536
42	1	0	5.149773	0.968960	0.363726
43	6	0	-2.914856	0.237139	0.645635
44	6	0	-3.999311	-0.278355	-0.066941
45	6	0	-5.069974	0.528642	-0.420975
46	6	0	-5.057799	1.870435	-0.058385
47	6	0	-3.993438	2.408244	0.647958
48	6	0	-2.926666	1.585239	0.992871
49	1	0	-4.005861	-1.322709	-0.349802
50	1	0	-5.908427	0.125082	-0.969430
51	1	0	-3.996691	3.453115	0.921374
52	1	0	-2.094360	2.004869	1.543654
53	17	0	3.695545	5.599562	0.228338

54	17	0	-6.406126	2.894985	-0.502908

Compound **3b** at **B3LYP-D3**/cc-pVTZ level.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.818384	0.811982	0.203526
2	6	0	2.497691	-1.084148	-0.111718
3	5	0	2.941660	0.011008	-1.333659
4	5	0	4.119203	1.240146	-0.744093
5	5	0	4.290829	0.962412	0.999840
6	5	0	3.161415	-0.385756	1.349872
7	5	0	3.676143	-1.617307	-1.184263
8	5	0	4.675762	-0.217781	-1.594417
9	5	0	5.513538	0.324575	-0.106908
10	5	0	4.901061	-0.679609	1.244259
11	5	0	3.779883	-1.886997	0.571443
12	5	0	5.225412	-1.396976	-0.362249
13	1	0	2.117044	0.261780	-2.141117
14	1	0	4.100899	2.319286	-1.222337
15	1	0	4.366074	1.848127	1.777776
16	1	0	2.497907	-0.406795	2.323745
17	1	0	3.340241	-2.462101	-1.935357
18	1	0	5.158242	-0.126878	-2.669242
19	1	0	6.598828	0.792342	-0.124572
20	1	0	5.541460	-0.943276	2.201745
21	1	0	3.551520	-2.927950	1.079197
22	1	0	6.106368	-2.162392	-0.548872
23	7	0	1.659867	1.534362	0.439541
24	7	0	1.183198	-1.493472	-0.132178
25	1	0	1.486264	1.705919	1.418056
26	1	0	0.644600	-1.142373	-0.906680
27	6	0	1.223099	2.619083	-0.435837
28	6	0	0.407791	-1.776378	1.075237
29	1	0	1.448107	2.326801	-1.460828
30	1	0	1.777621	3.542873	-0.243643
31	1	0	0.326802	-0.895691	1.715420
32	1	0	0.935736	-2.544095	1.643795
33	6	0	-0.260474	2.860281	-0.284731
34	6	0	-1.159778	1.796425	-0.368585
35	6	0	-2.525813	1.999827	-0.253503

36	6	0	-3.002537	3.289421	-0.048202
37	6	0	-2.131543	4.364712	0.041553
38	6	0	-0.763607	4.140624	-0.075834
39	1	0	-0.785747	0.793188	-0.513936
40	1	0	-3.214542	1.170730	-0.323476
41	1	0	-2.516913	5.359962	0.206942
42	1	0	-0.083665	4.979678	-0.000337
43	6	0	-0.971247	-2.245643	0.690979
44	6	0	-1.145030	-3.431174	-0.024314
45	6	0	-2.409442	-3.855735	-0.404669
46	6	0	-3.514774	-3.083350	-0.065726
47	6	0	-3.369123	-1.901074	0.644806
48	6	0	-2.094112	-1.489372	1.016262
49	1	0	-0.280317	-4.024925	-0.290214
50	1	0	-2.543079	-4.774669	-0.956139
51	1	0	-4.238069	-1.313130	0.901688
52	1	0	-1.977700	-0.563255	1.563574
53	17	0	-4.726578	3.554747	0.106696
54	17	0	-5.113455	-3.611268	-0.544420

Compound **3b** at **B3PW91**/cc-pVTZ level.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.493043	-2.214456	0.143718
2	6	0	-0.410577	-2.391771	-0.087200
3	5	0	0.694575	-2.644198	-1.337476
4	5	0	2.195921	-3.431806	-0.743962
5	5	0	2.048000	-3.545382	1.015398
6	5	0	0.486491	-2.759161	1.373825
7	5	0	-0.677437	-3.749198	-1.051307
8	5	0	0.900969	-4.398697	-1.473532
9	5	0	1.696008	-4.959702	0.023575
10	5	0	0.628665	-4.520199	1.387168
11	5	0	-0.837773	-3.777967	0.715741
12	5	0	-0.048822	-5.125517	-0.148443
13	1	0	0.708655	-1.844232	-2.211002
14	1	0	3.217316	-3.190316	-1.289515
15	1	0	2.961060	-3.339646	1.741320
16	1	0	0.329750	-2.043774	2.303160
17	1	0	-1.615614	-3.685263	-1.768034

18	1	0	1.072997	-4.918584	-2.523712
19	1	0	2.425703	-5.892788	0.041418
20	1	0	0.565982	-5.133483	2.398526
21	1	0	-1.884758	-3.781810	1.268034
22	1	0	-0.583347	-6.179305	-0.232643
23	7	0	1.931295	-0.901390	0.252859
24	7	0	-1.155177	-1.241518	-0.146968
25	1	0	2.068084	-0.620265	1.212904
26	1	0	-0.951084	-0.637450	-0.926227
27	6	0	2.977214	-0.398099	-0.636304
28	6	0	-1.735375	-0.592738	1.016013
29	1	0	2.664940	-0.596033	-1.663434
30	1	0	3.925500	-0.925026	-0.483714
31	1	0	-0.995574	-0.007293	1.572322
32	1	0	-2.089475	-1.378539	1.687003
33	6	0	3.183419	1.077849	-0.428453
34	6	0	2.179890	1.991963	-0.745315
35	6	0	2.365026	3.351466	-0.559538
36	6	0	3.572524	3.806715	-0.046589
37	6	0	4.586457	2.920883	0.277226
38	6	0	4.382194	1.560964	0.084178
39	1	0	1.238662	1.635684	-1.146358
40	1	0	1.586135	4.057804	-0.813206
41	1	0	5.521941	3.290038	0.674996
42	1	0	5.176256	0.866882	0.335197
43	6	0	-2.883194	0.300273	0.621392
44	6	0	-3.927526	-0.181947	-0.166011
45	6	0	-4.996425	0.629715	-0.507540
46	6	0	-5.023795	1.942248	-0.055896
47	6	0	-3.998127	2.446233	0.726546
48	6	0	-2.932515	1.619858	1.056617
49	1	0	-3.902454	-1.205946	-0.518671
50	1	0	-5.806261	0.251688	-1.116768
51	1	0	-4.031116	3.471857	1.068173
52	1	0	-2.127421	2.014677	1.666065
53	17	0	3.812533	5.511684	0.189463
54	17	0	-6.361656	2.966886	-0.482348

Compound **3b** at **B3PW91-D3**/cc-pVTZ level.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	2.824925	0.768304	0.239247
2	6	0	2.487900	-1.054366	-0.133543
3	5	0	2.943757	0.062433	-1.327954
4	5	0	4.134488	1.238322	-0.687760
5	5	0	4.300258	0.884191	1.036781
6	5	0	3.170205	-0.465019	1.345061
7	5	0	3.641893	-1.578168	-1.237645
8	5	0	4.670062	-0.185245	-1.600061
9	5	0	5.516524	0.283655	-0.096824
10	5	0	4.903504	-0.769592	1.210250
11	5	0	3.760889	-1.926924	0.496415
12	5	0	5.203245	-1.422137	-0.424332
13	1	0	2.112498	0.353716	-2.120439
14	1	0	4.119446	2.344583	-1.110126
15	1	0	4.380704	1.742155	1.850036
16	1	0	2.509196	-0.512733	2.324209
17	1	0	3.277869	-2.389425	-2.017777
18	1	0	5.146541	-0.058365	-2.677782
19	1	0	6.609858	0.741867	-0.097281
20	1	0	5.545416	-1.078650	2.157441
21	1	0	3.505937	-2.988798	0.953982
22	1	0	6.072079	-2.195724	-0.651833
23	7	0	1.678715	1.492853	0.513980
24	7	0	1.168689	-1.446686	-0.168084
25	1	0	1.530779	1.641529	1.500006
26	1	0	0.642435	-1.055756	-0.932397
27	6	0	1.251256	2.602404	-0.319611
28	6	0	0.392277	-1.703141	1.034426
29	1	0	1.507044	2.358046	-1.351974
30	1	0	1.789109	3.525941	-0.077282
31	1	0	0.313856	-0.813008	1.665663
32	1	0	0.913400	-2.467677	1.617012
33	6	0	-0.235420	2.822155	-0.206949
34	6	0	-1.113804	1.741424	-0.208436
35	6	0	-2.483758	1.929580	-0.144131
36	6	0	-2.985700	3.221728	-0.073372
37	6	0	-2.133702	4.315008	-0.066006
38	6	0	-0.762957	4.105961	-0.130872
39	1	0	-0.719252	0.735095	-0.248530
40	1	0	-3.157050	1.083183	-0.150252
41	1	0	-2.539584	5.315424	-0.003208
42	1	0	-0.097252	4.961531	-0.119166
43	6	0	-0.986698	-2.168589	0.658786

44	6	0	-1.162774	-3.262196	-0.186765
45	6	0	-2.430957	-3.685574	-0.547803
46	6	0	-3.538597	-3.007132	-0.056163
47	6	0	-3.389467	-1.917942	0.787597
48	6	0	-2.111157	-1.505025	1.136360
49	1	0	-0.294451	-3.783500	-0.571373
50	1	0	-2.566923	-4.534561	-1.203769
51	1	0	-4.261799	-1.399089	1.161151
52	1	0	-1.992353	-0.646424	1.786720
53	17	0	-4.704334	3.469023	0.016614
54	17	0	-5.132822	-3.529357	-0.508997

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(4) References

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