Supporting Information

Contents

NMR spectra

1,8-Diiodonaphthalene

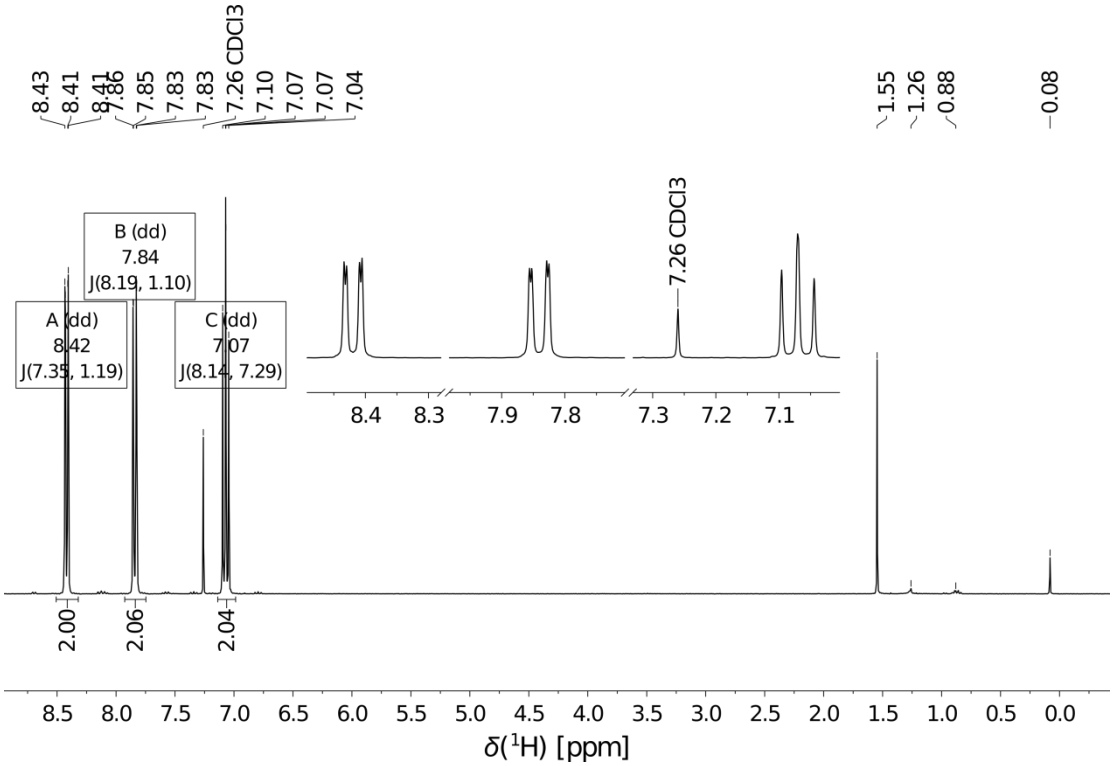


Figure S1. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 1,8-diiodonaphthalene.

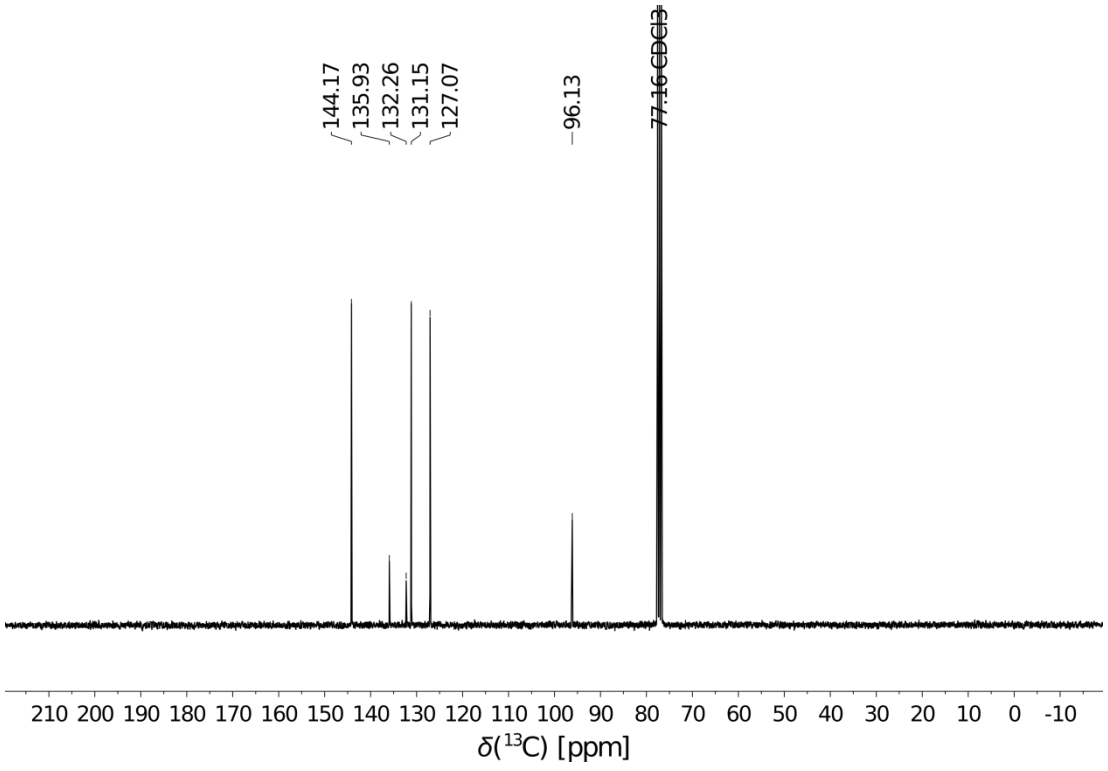


Figure S2. Full $^{13}C\{^{1}H\}$ NMR spectrum (75 MHz, $CDCl_3$) of 1,8-diiodonaphthalene.

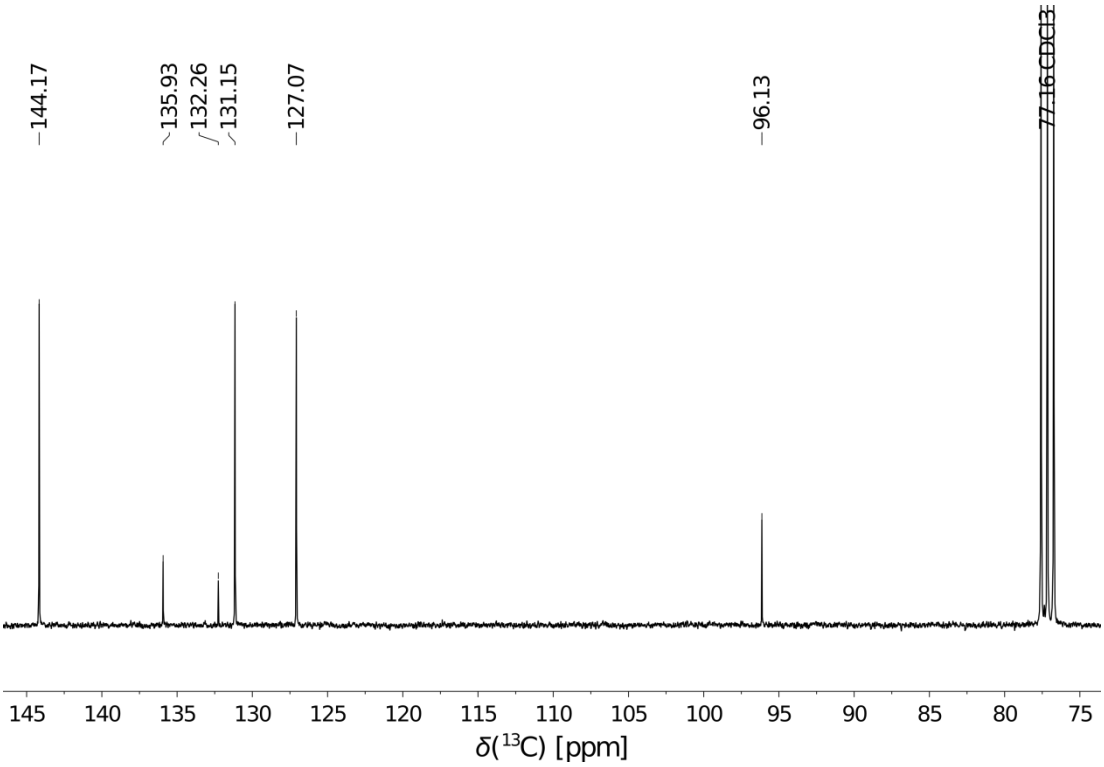


Figure S3. Excerpt of the $^{13}C\{^{1}H\}$ NMR spectrum (75 MHz, $CDCl_3$) of 1,8-diiodonaphthalene.

1,8-Bis(diisopropoxyboranyl)naphthalene

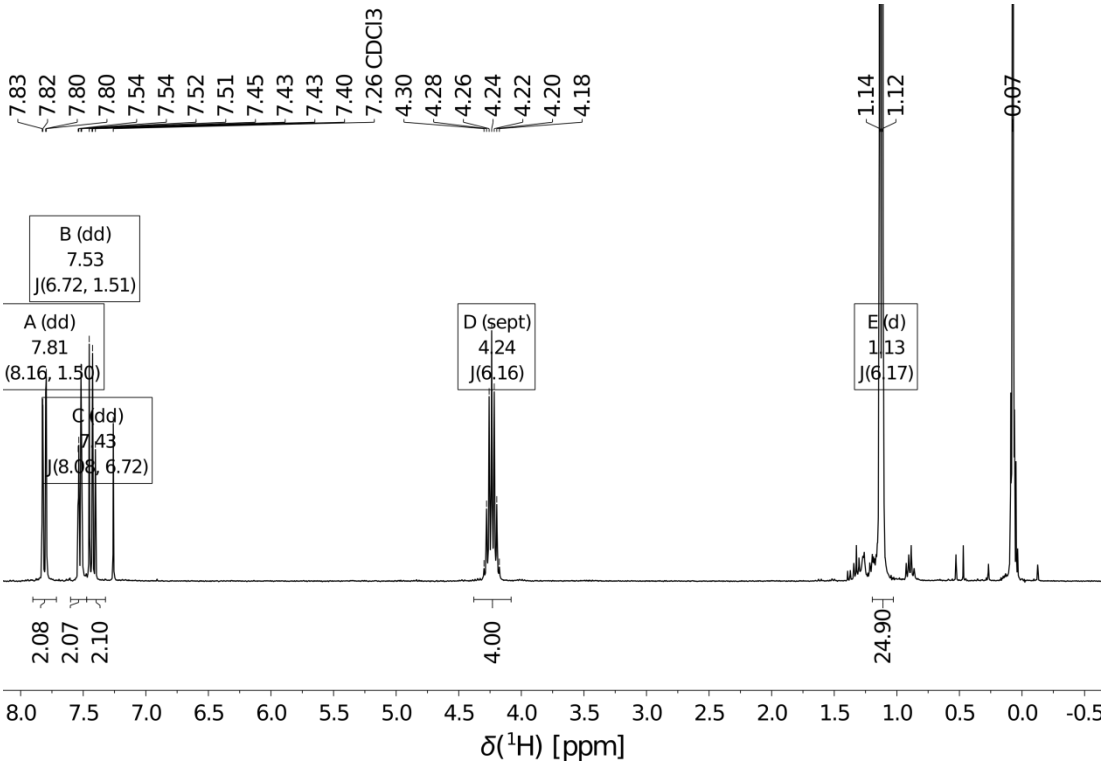


Figure S4. Full ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 1,8-bis(diisopropoxyboranyl)naphthalene.

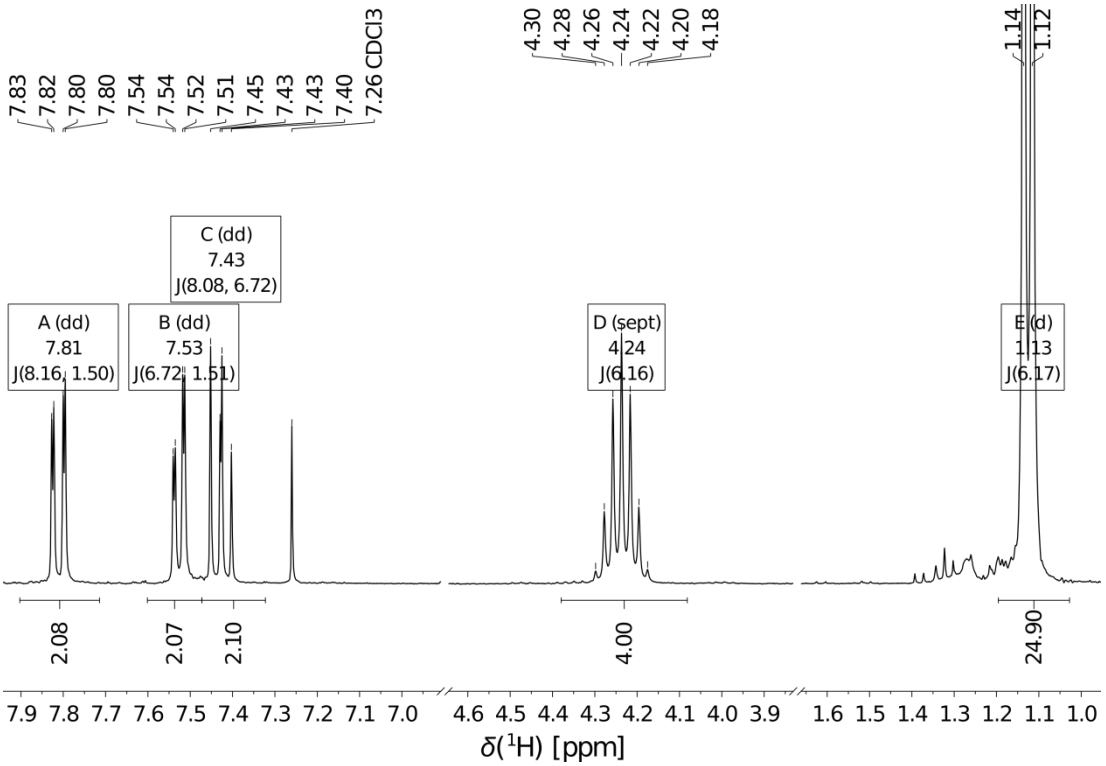


Figure S5. Excerpts of the ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 1,8-bis(diisopropoxyboranyl)naphthalene.

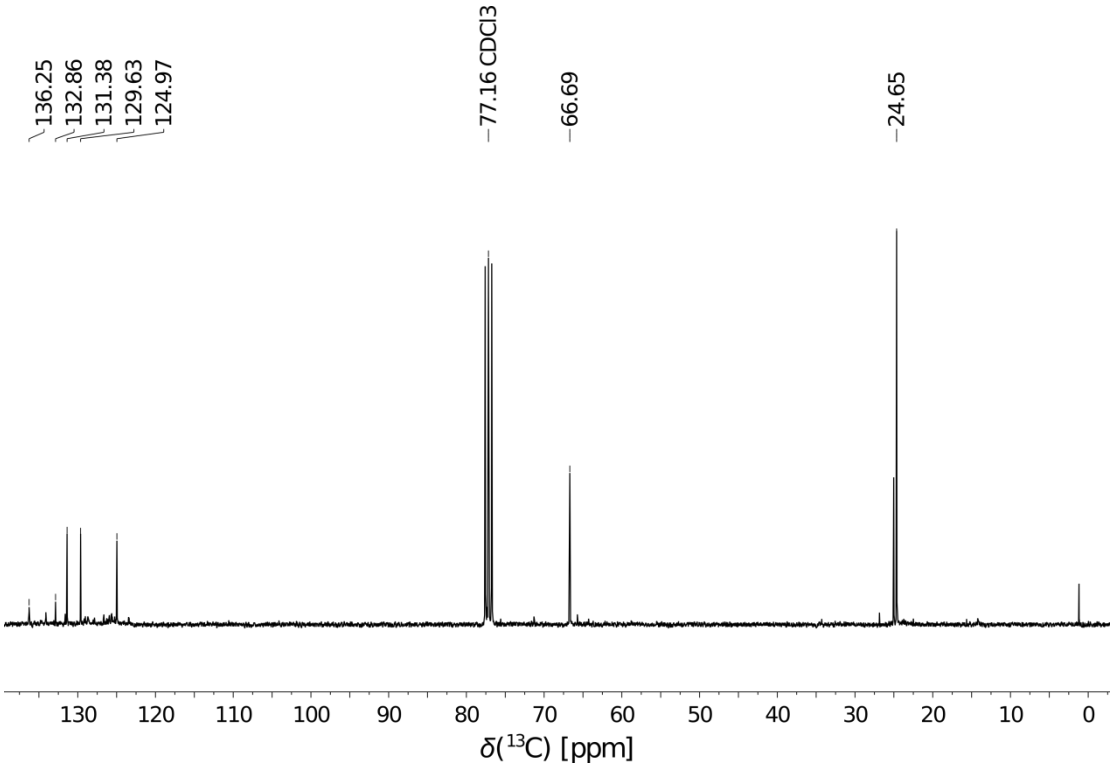


Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum (75 MHz, $CDCl_3$) of 1,8-bis(diisopropoxyboranyl)naphthalene.

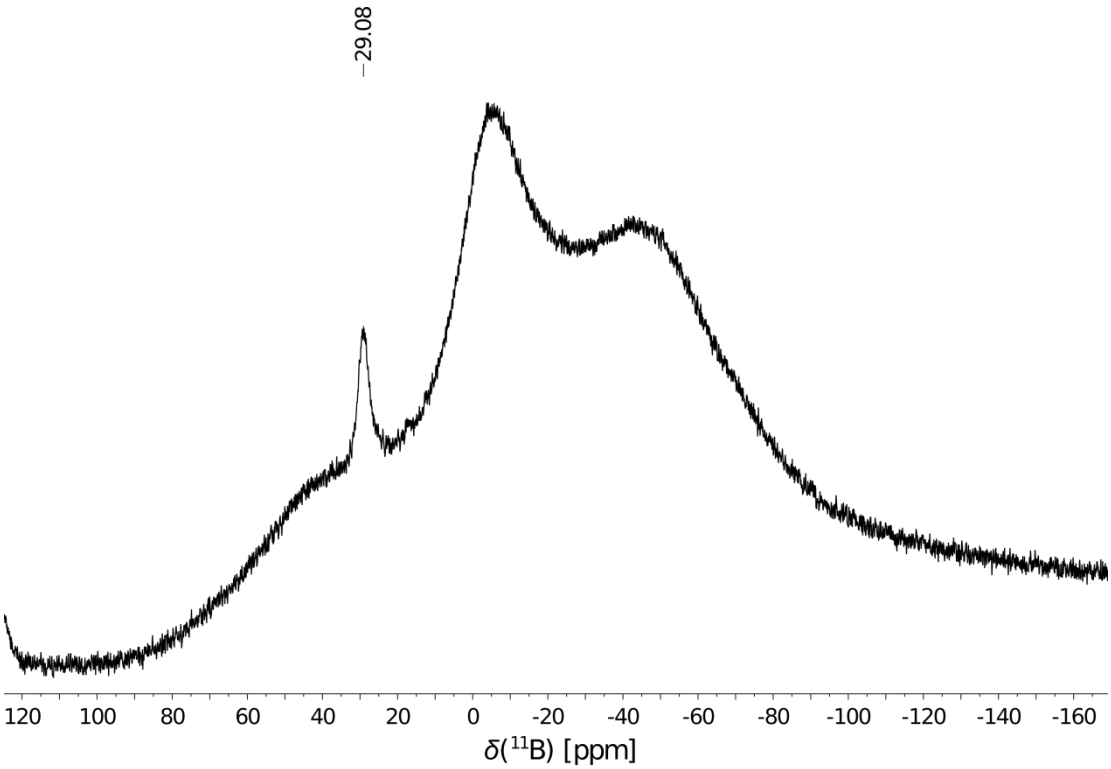


Figure S7. ^{11}B NMR spectrum (96 MHz, $CDCl_3$) of 1,8-bis(diisopropoxyboranyl)naphthalene.

1,8-Bis(dimethylboranyl)naphthalene (1)

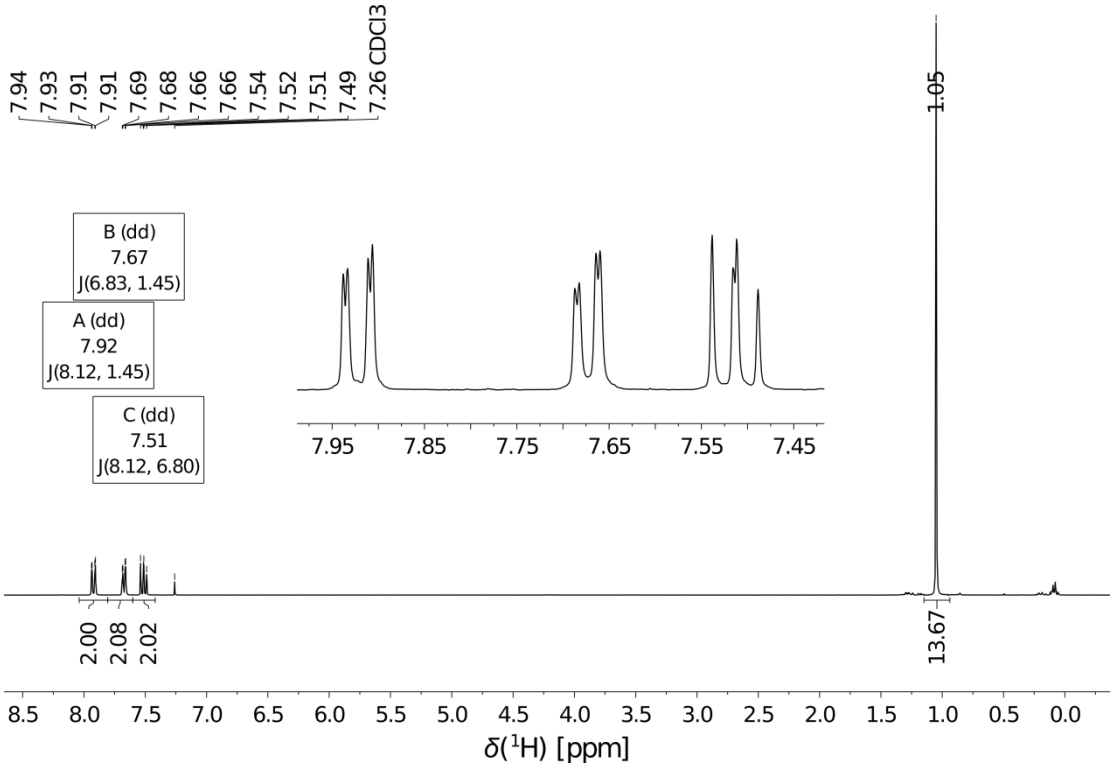


Figure S8. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 1,8-bis(dimethylboranyl)naphthalene.

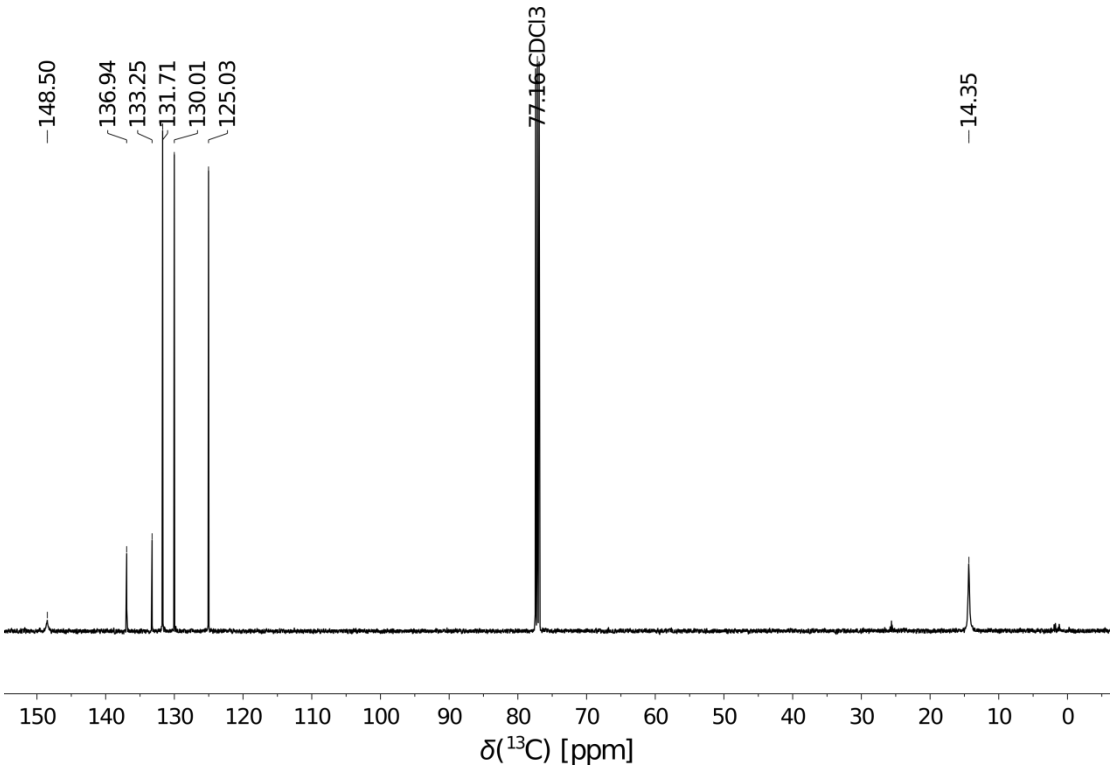


Figure S9. $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, $CDCl_3$) of 1,8-bis(dimethylboranyl)naphthalene.

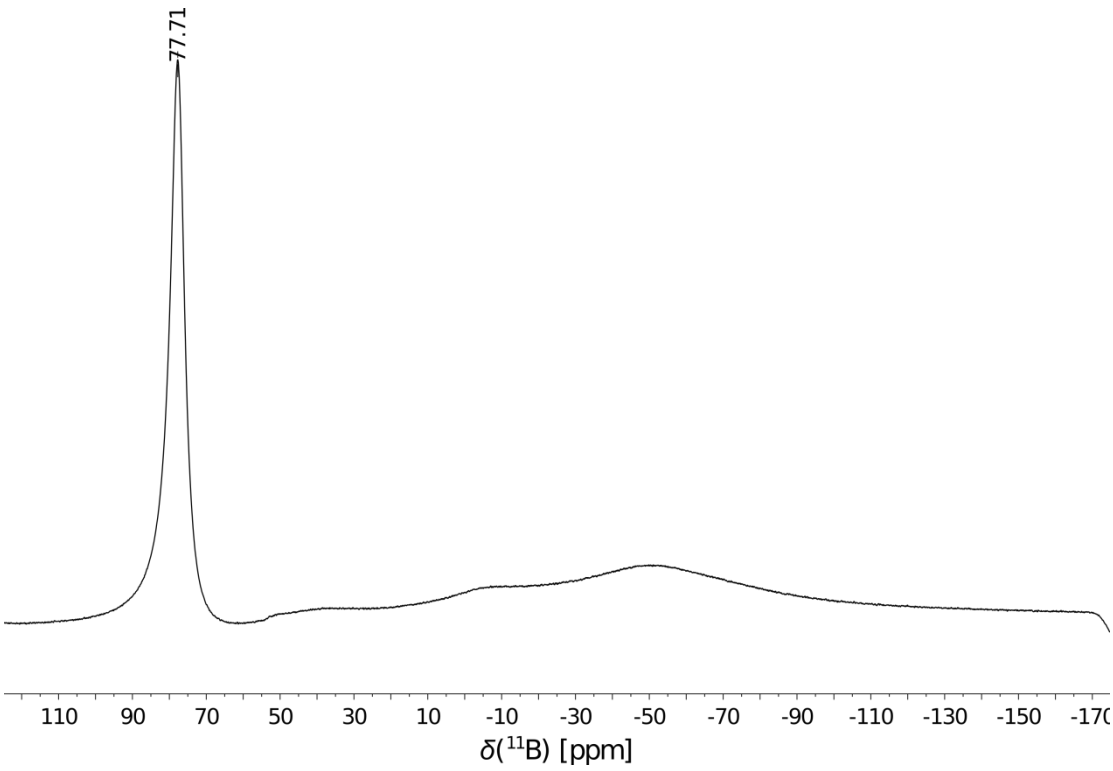


Figure S10. ^{11}B NMR spectrum (96 MHz, $CDCl_3$) of 1,8-bis(dimethylboranyl)naphthalene.

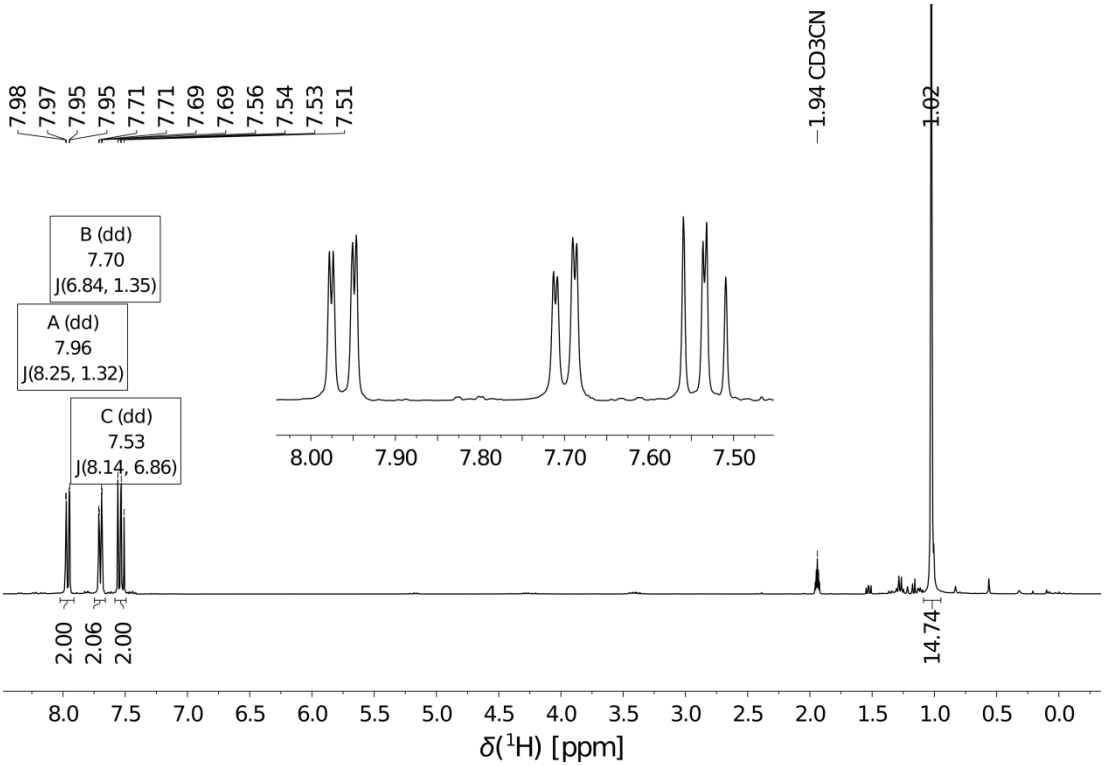


Figure S11. ^{1}H NMR spectrum (300 MHz, CD_3CN) of 1,8-bis(dimethylboranyl)naphthalene.

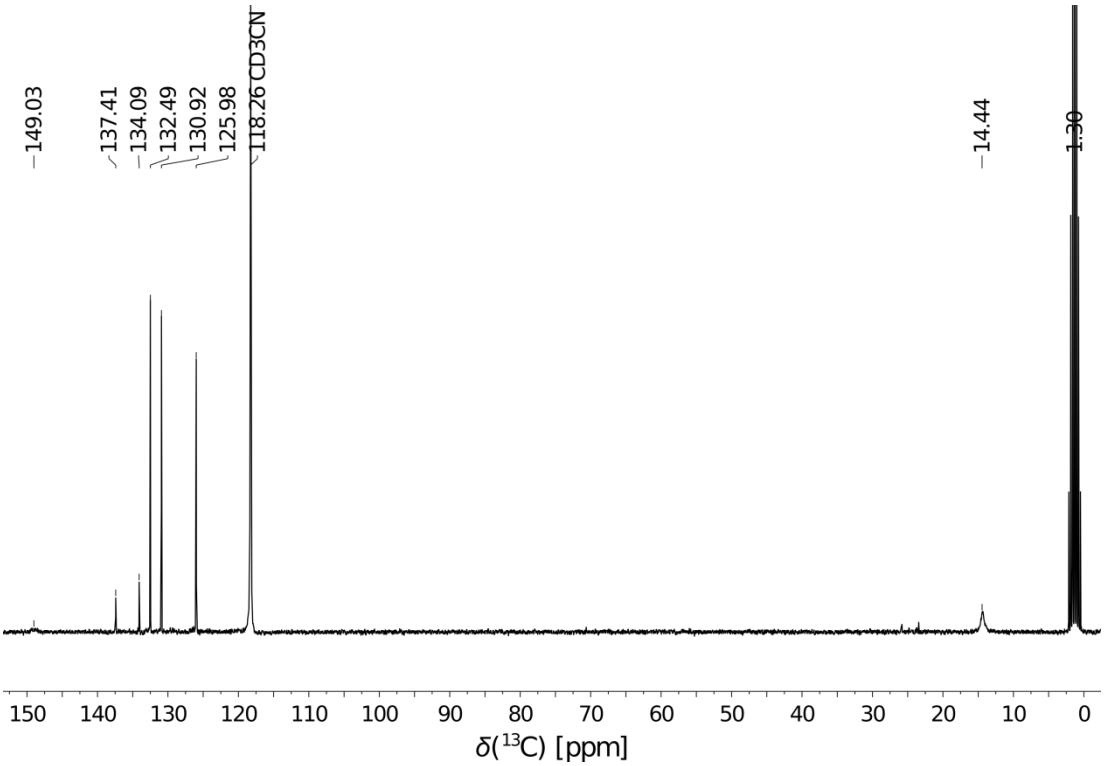


Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum (75 MHz, CD_3CN) of 1,8-bis(dimethylboranyl)naphthalene.

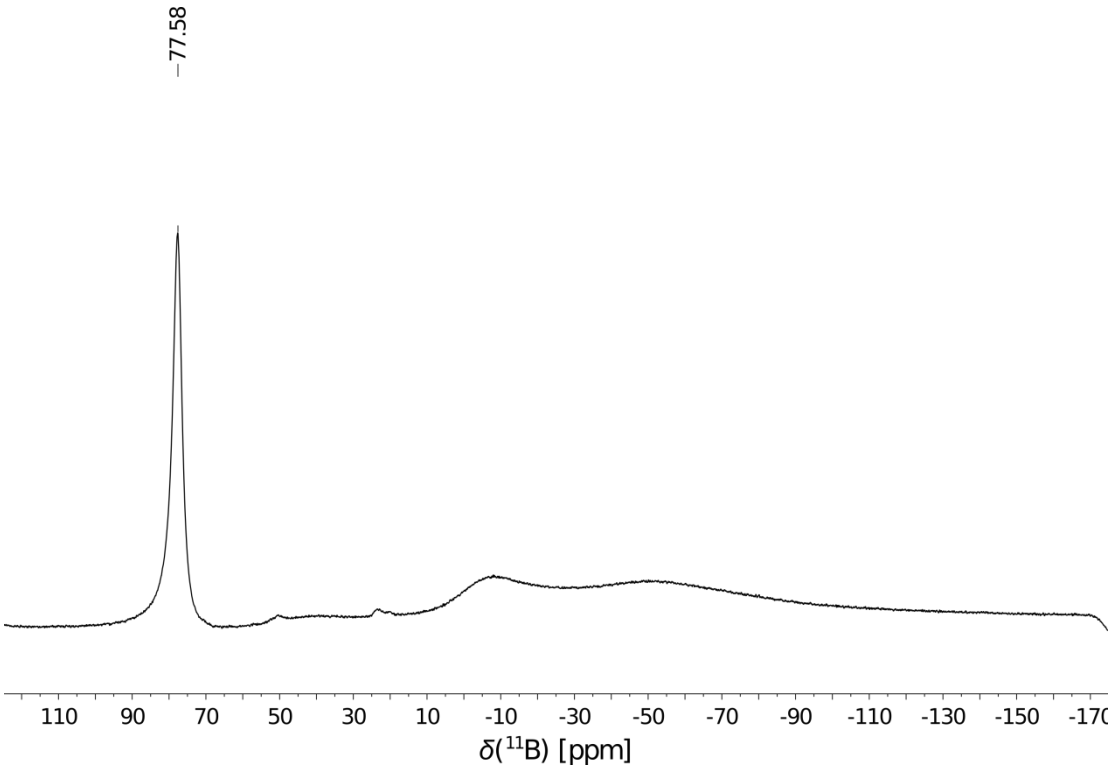


Figure S13. ^{11}B NMR spectrum (96 MHz, CD_3CN) of 1,8-bis(dimethylboranyl)naphthalene.

[1-OH][3-H]

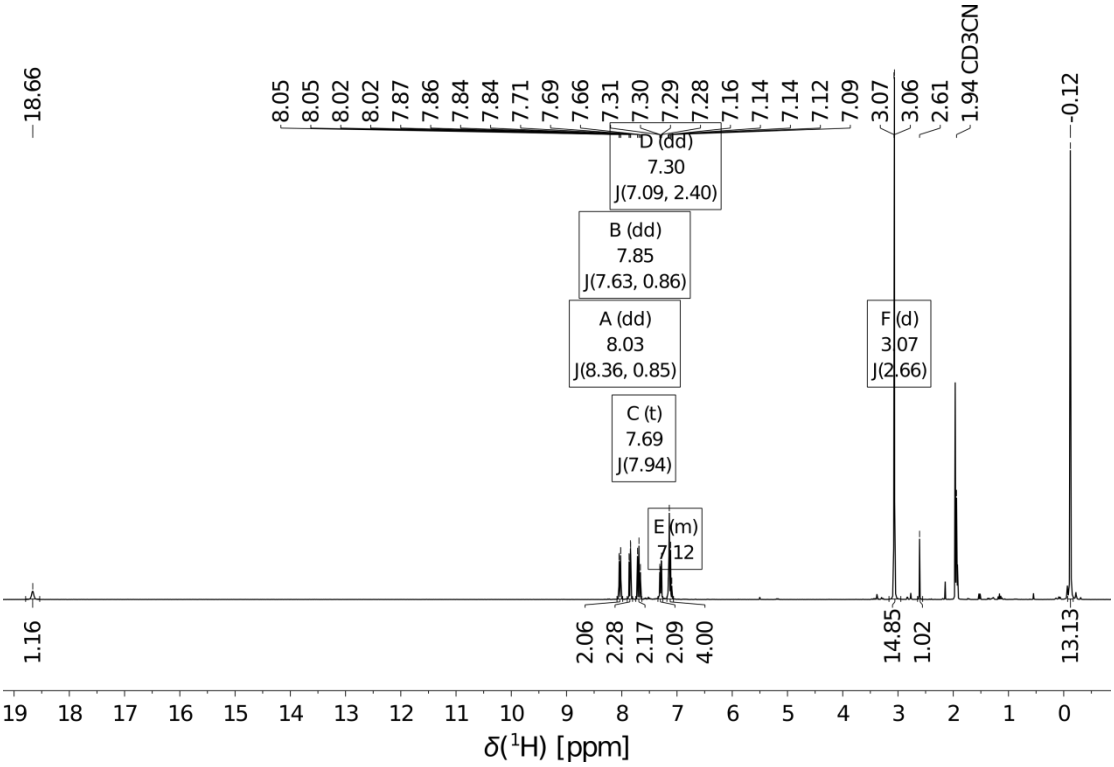


Figure S14. Full ^{1}H NMR spectrum (300 MHz, CD_3CN) of [**1**-OH][**3**-H].

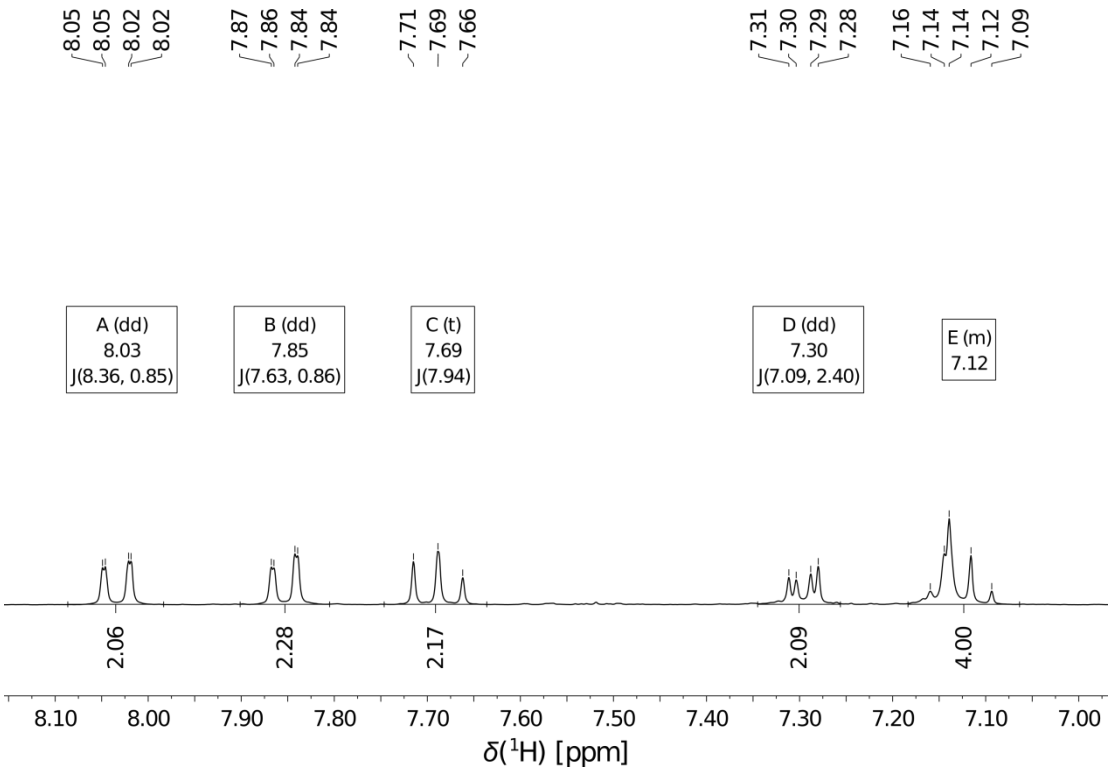


Figure S15. Excerpt of the ^{1}H NMR spectrum (300 MHz, CD_3CN) of [**1**-OH][**3**-H] containing the signals of protons bound to the naphthalene backbones.

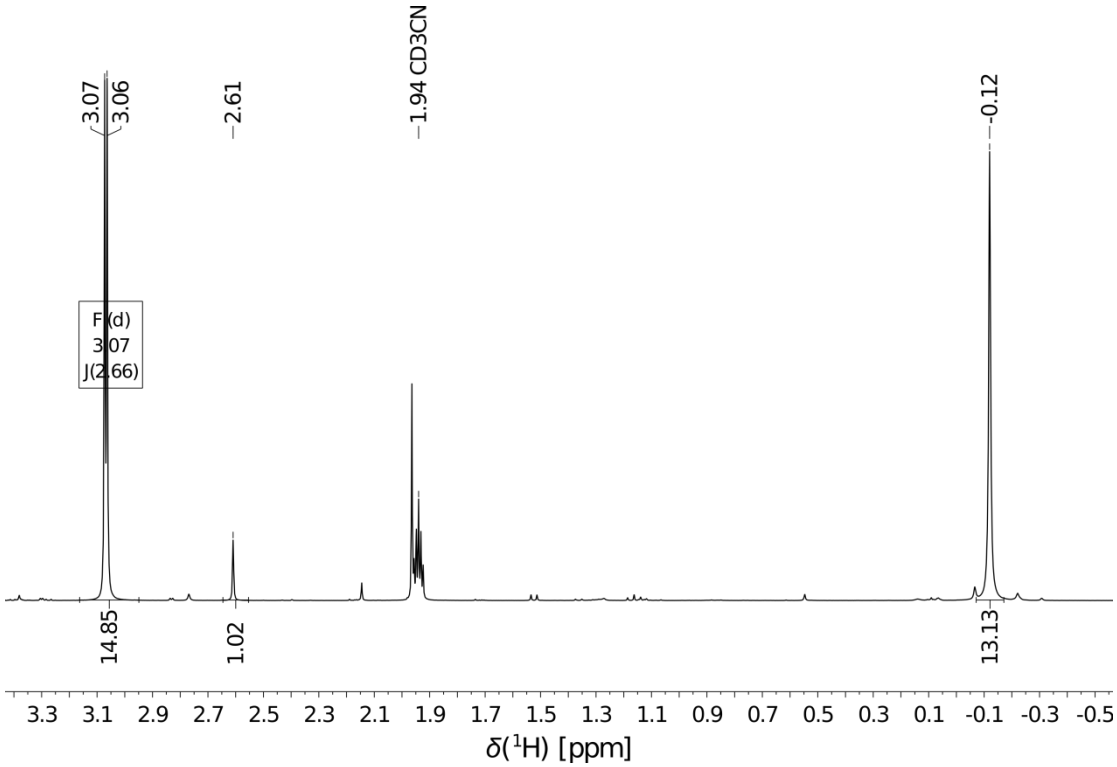


Figure S16. Excerpt of the ^{1}H NMR spectrum (300 MHz, CD_3CN) of [**1**-OH][**3**-H] containing the signals of protons of the methyl groups as well as O*H*. The peak to the side of the solvent signal is due to traces of CH_3CN.

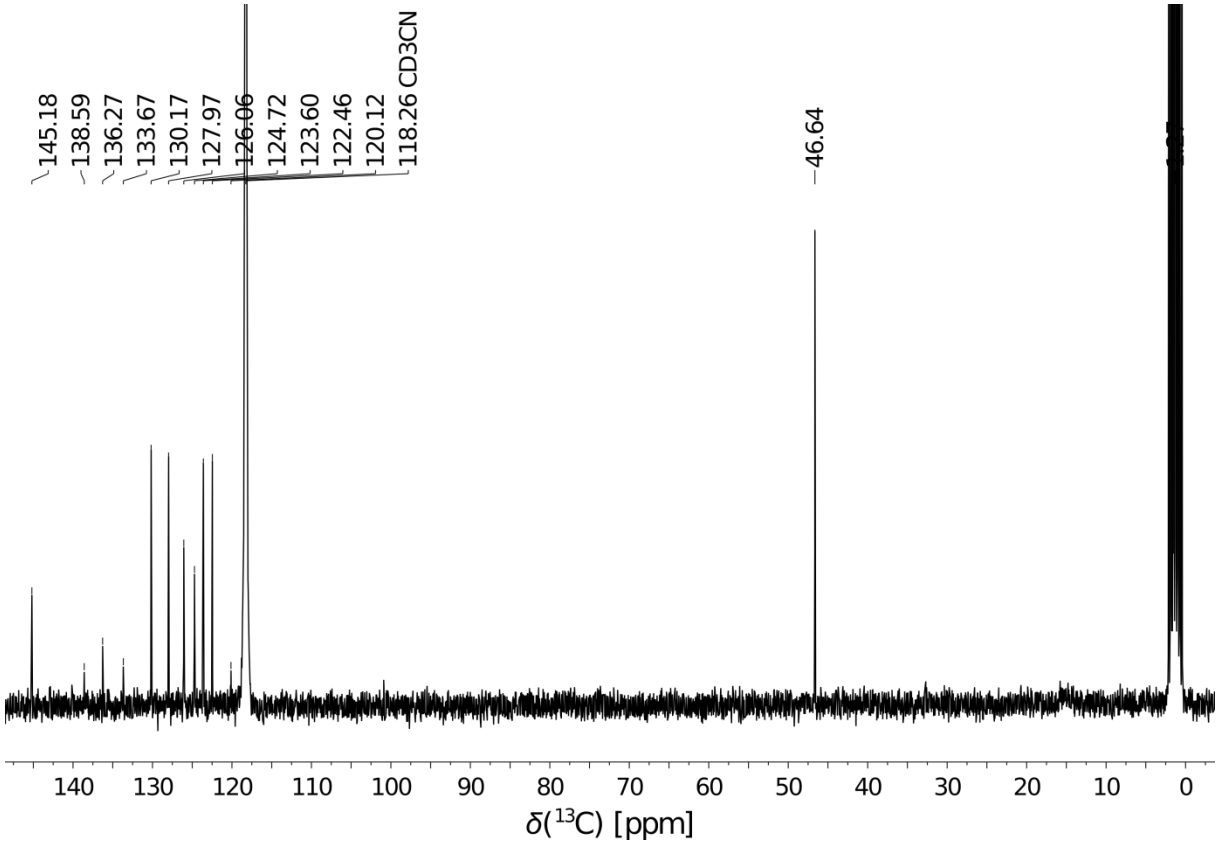


Figure S17. Full $^{13}C\{^{1}H\}$ NMR spectrum (75 MHz, CD_3CN) of [**1**-OH][**3**-H].

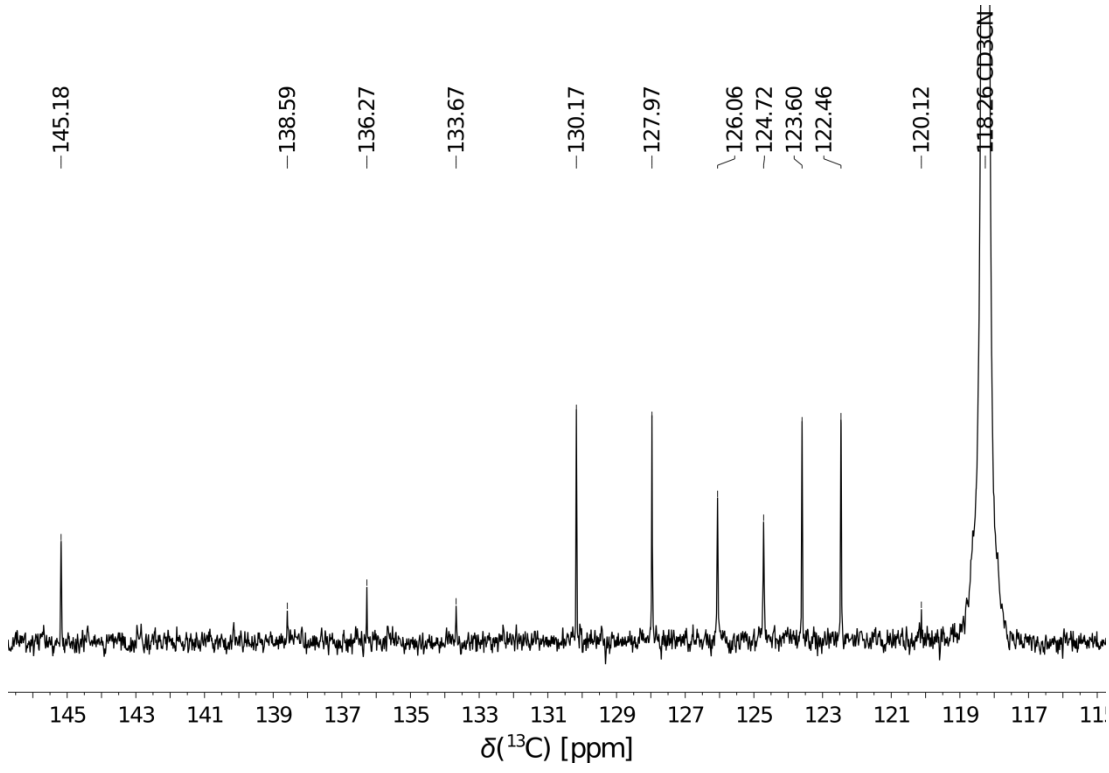


Figure S18. Excerpt of the $^{13}C\{^{1}H\}$ NMR spectrum (75 MHz, CD_3CN) of [**1**-OH][**3**-H].

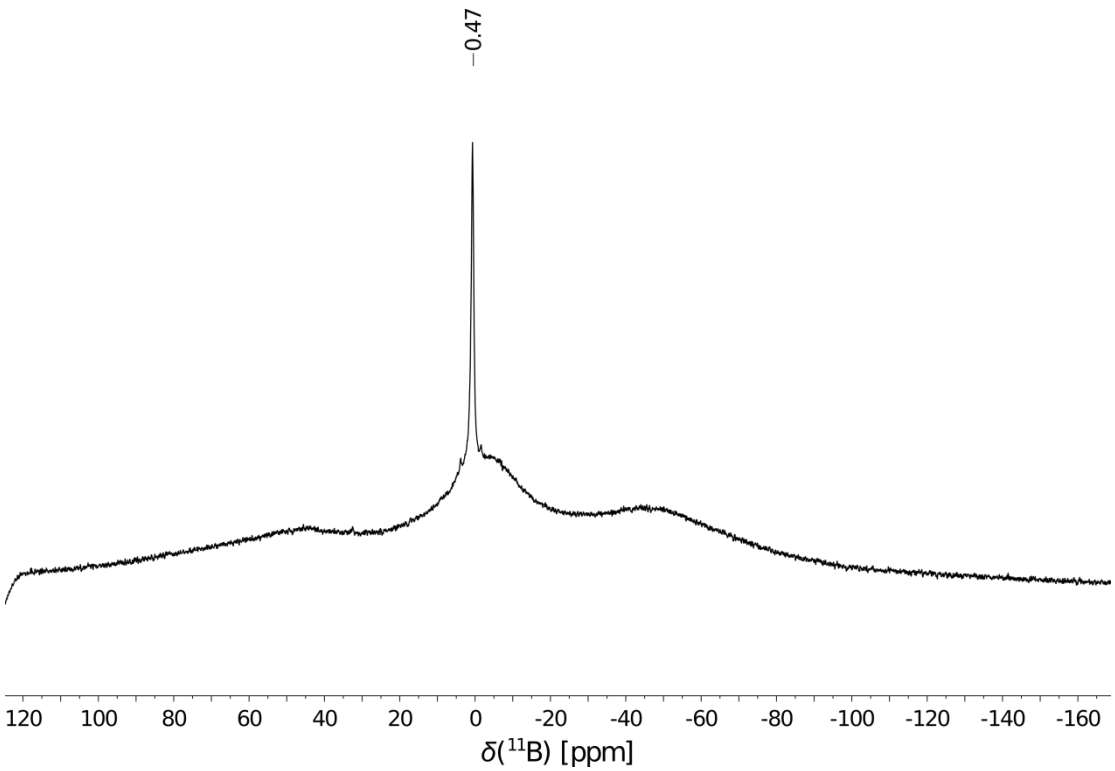


Figure S19. ^{11}B NMR spectrum (96 MHz, CD_3CN) of [**1**-OH][**3**-H].

[1-NH$_2$][3-H]

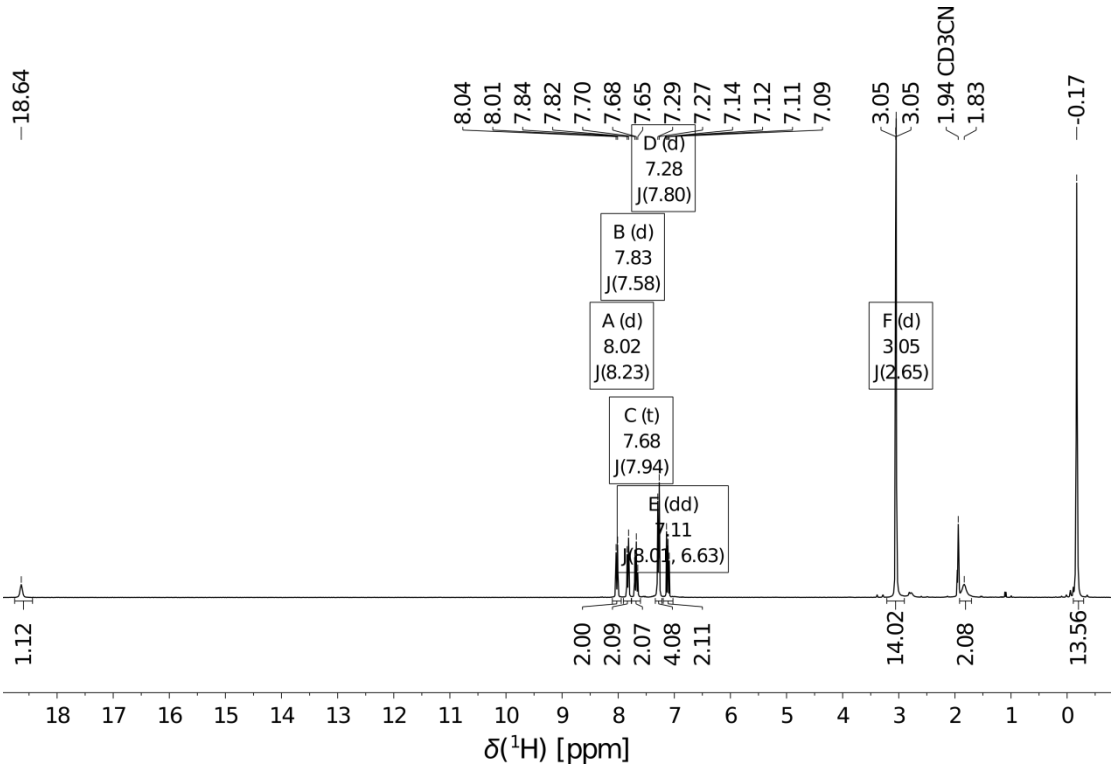


Figure S20. Full ^{1}H NMR spectrum (300 MHz, CD_3CN) of [**1**-NH$_2$][**3**-H].

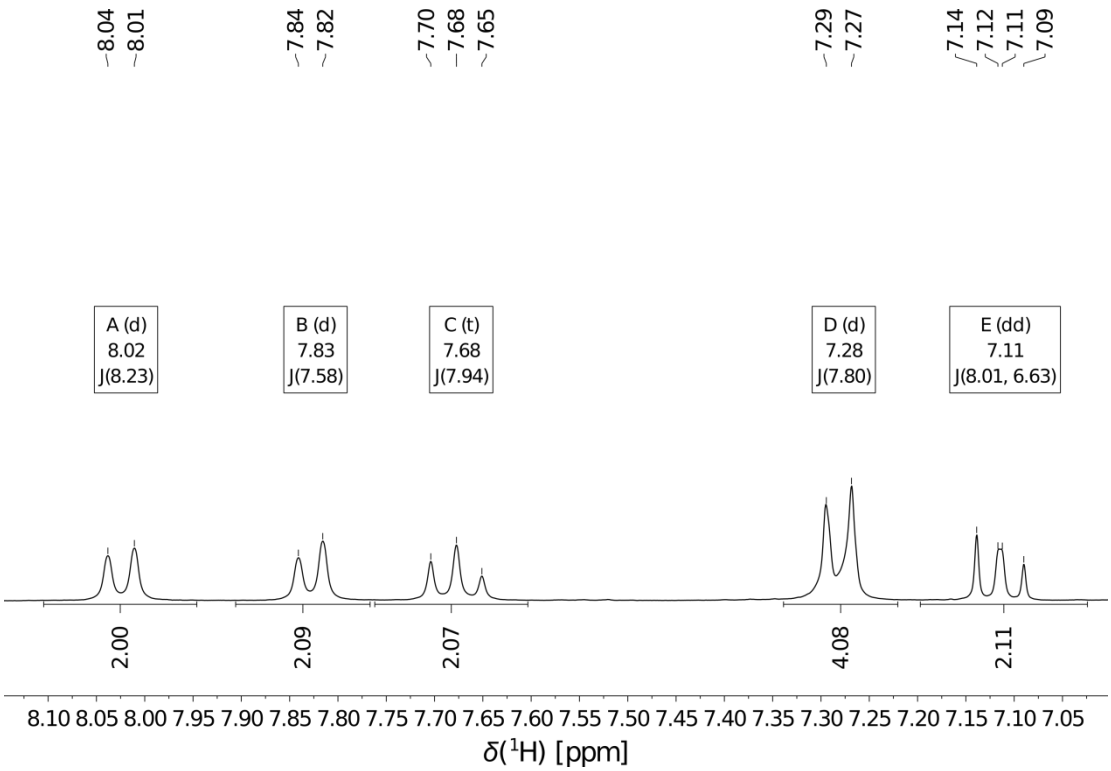


Figure S21. Excerpt of the ^{1}H NMR spectrum (300 MHz, CD_3CN) of [**1**-NH_2][**3**-H] containing the signals of protons bound to the naphthalene backbones.

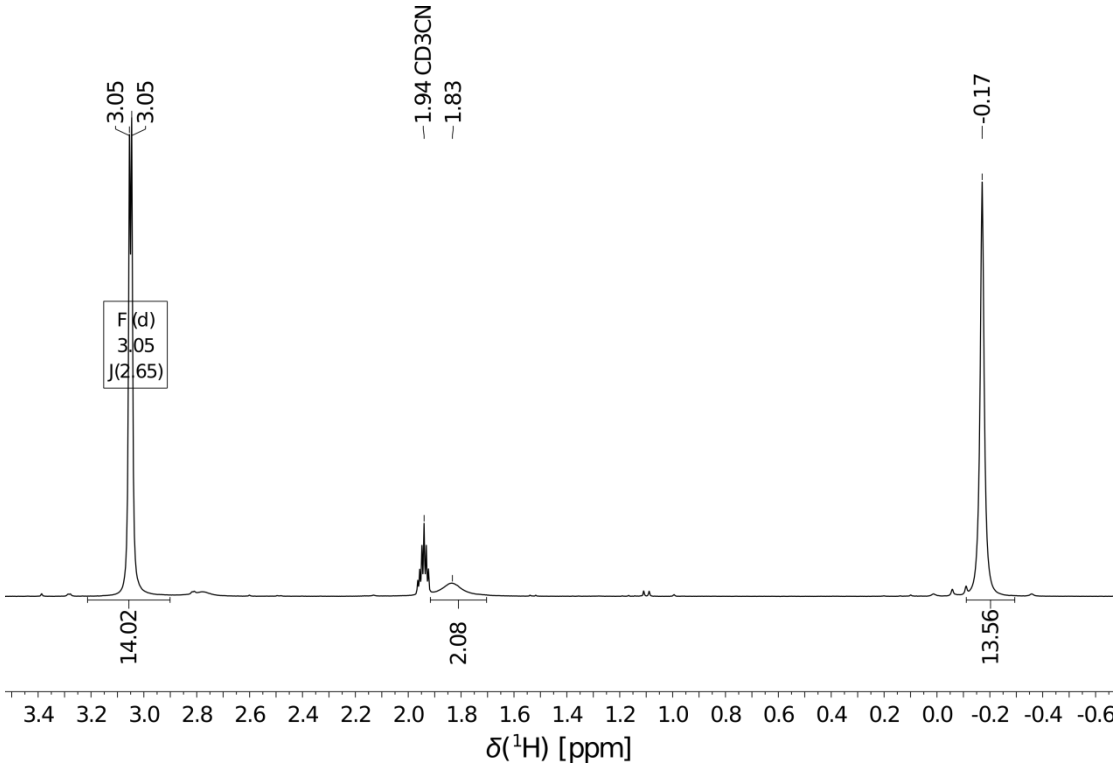


Figure S22. Excerpt of the ^{1}H NMR spectrum (300 MHz, CD_3CN) of [**1**-NH_2][**3**-H] containing the signals of the protons of the methyl groups as well as N*H*$_2$.

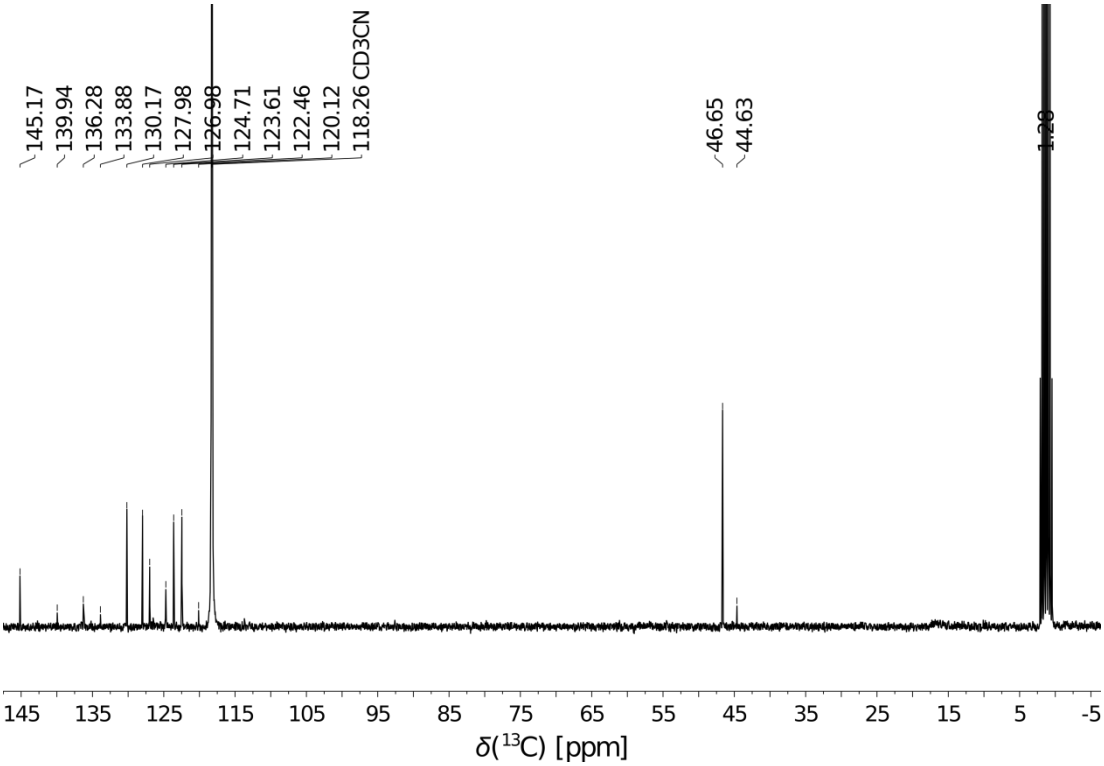


Figure S23. Full $^{13}C\{^{1}H\}$ NMR spectrum (75 MHz, CD_3CN) of [**1**-NH_2][**3**-H].

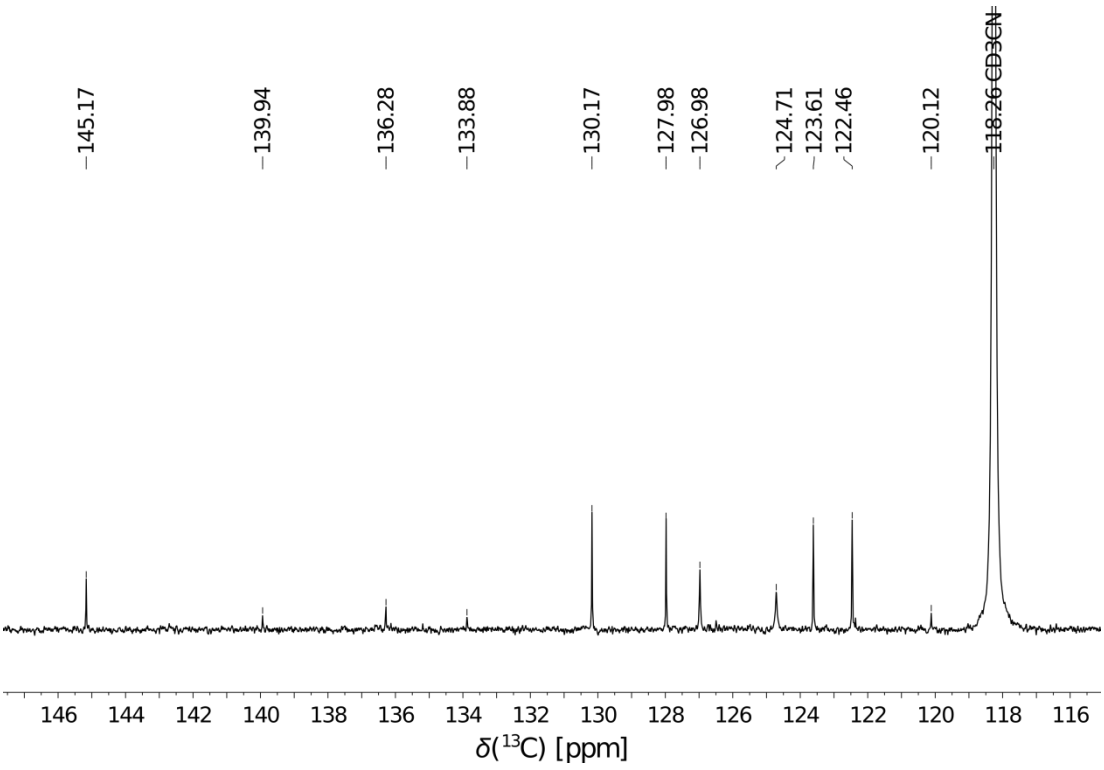


Figure S23. Excerpt of the $^{13}C\{^{1}H\}$ NMR spectrum (75 MHz, CD_3CN) of [**1**-NH_2][**3**-H].

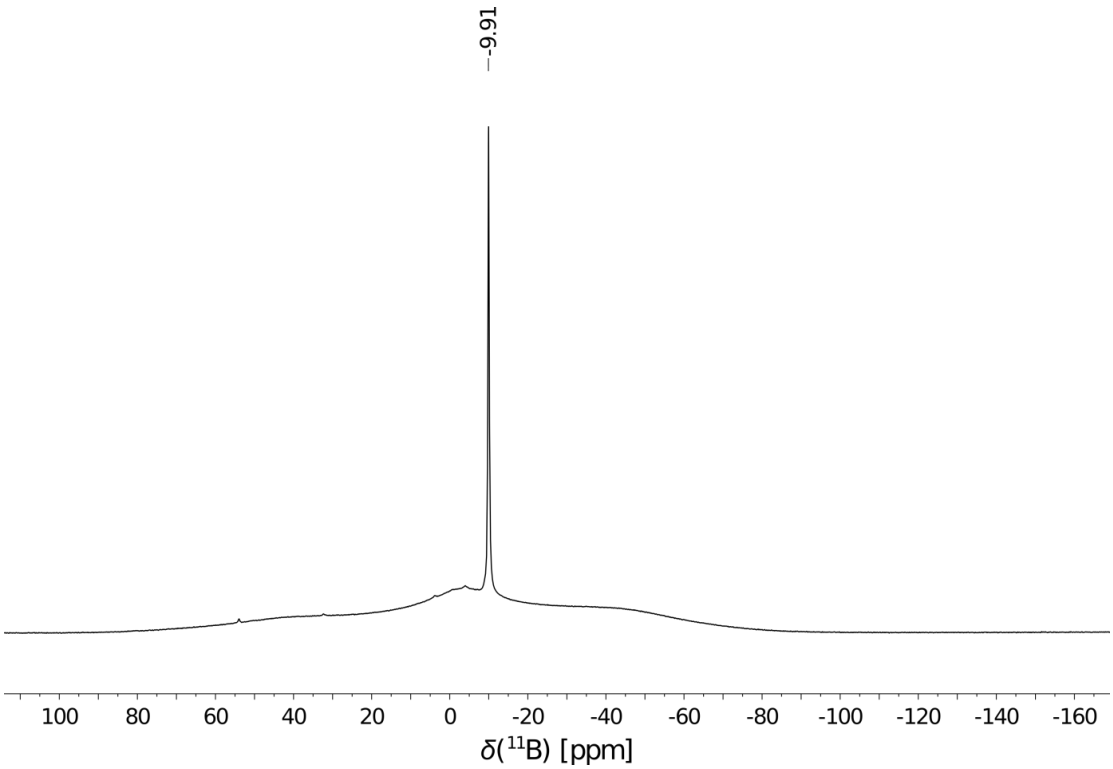


Figure S25. ^{11}B NMR spectrum (96 MHz, CD_3CN) of [**1**-NH_2][**3**-H].

[1-SH][3-H]

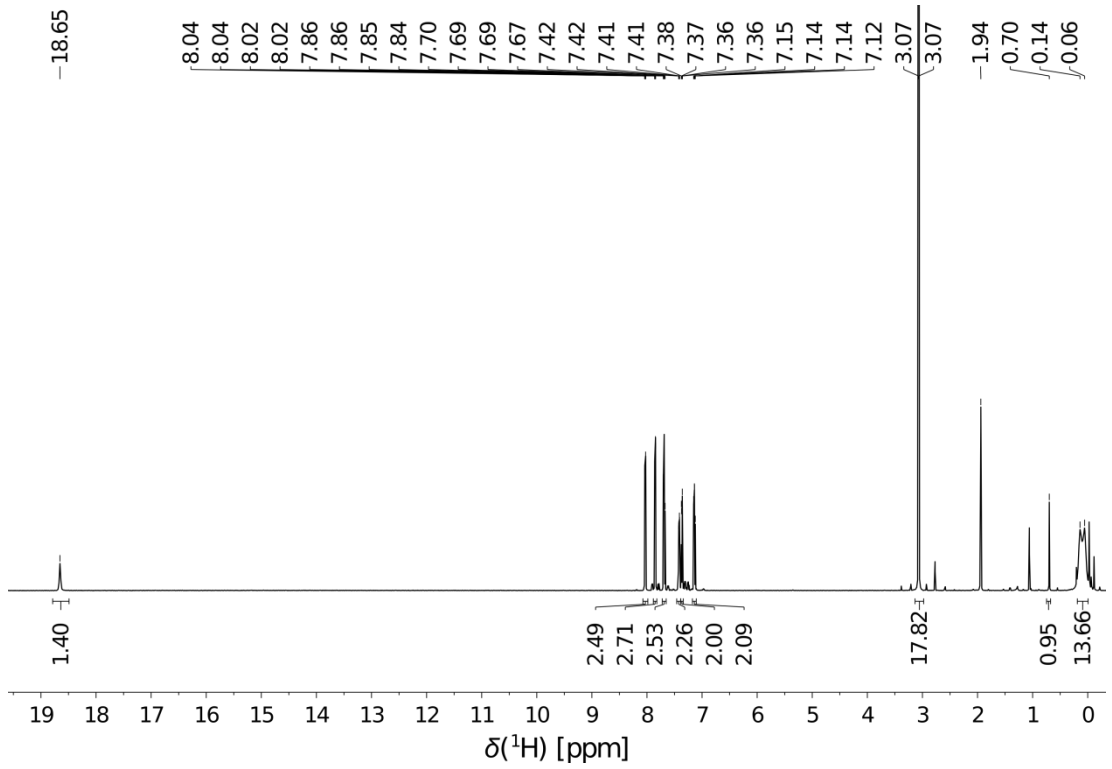


Figure S26. Full ^1H NMR spectrum (300 MHz, CD_3CN) of [**1**-SH][**3**-H].

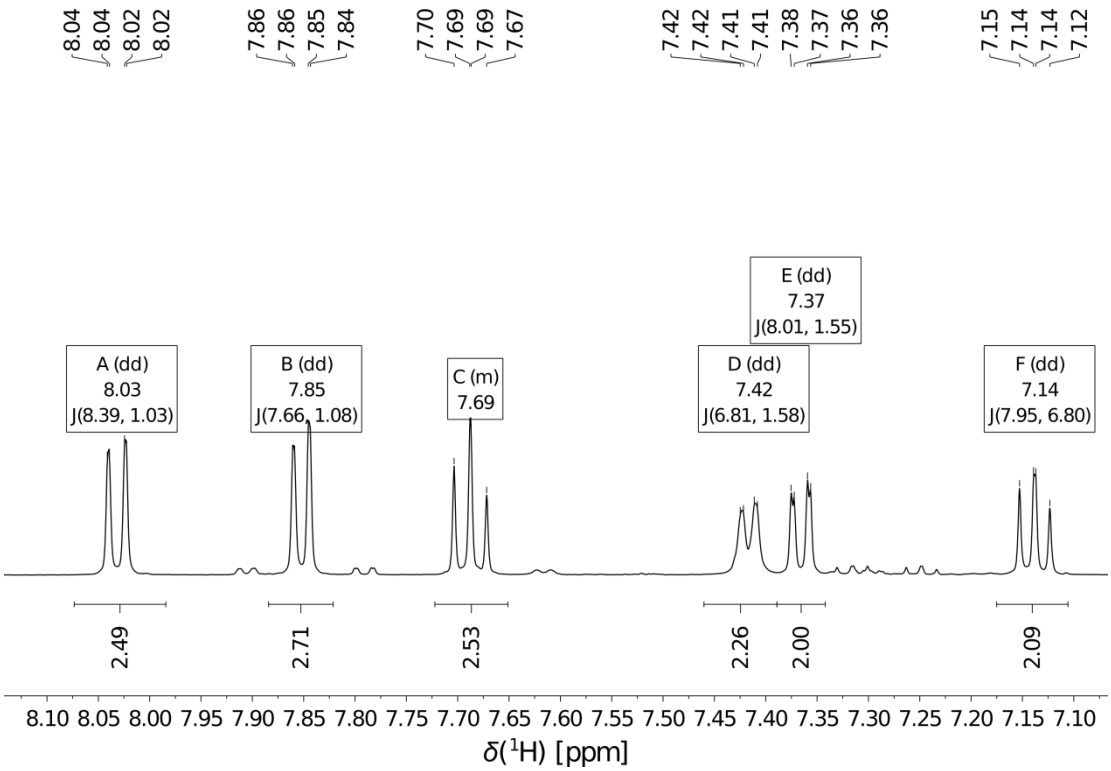


Figure S27. Excerpt of the ^{1}H NMR spectrum (300 MHz, CD_3CN) of [**1**-SH][**3**-H] containing the signals of protons bound to the naphthalene backbones.

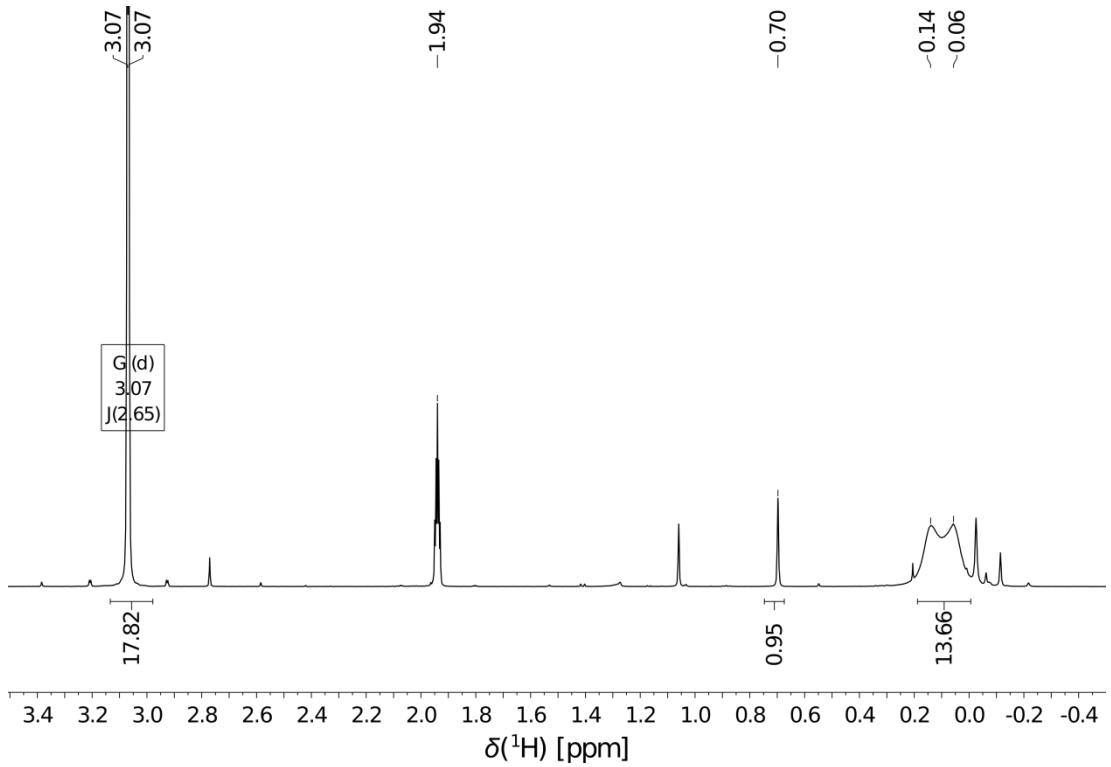


Figure S28. Excerpt of the ^{1}H NMR spectrum (300 MHz, CD_3CN) of [**1**-SH][**3**-H] containing the signals of the protons of the methyl groups as well as S*H*.

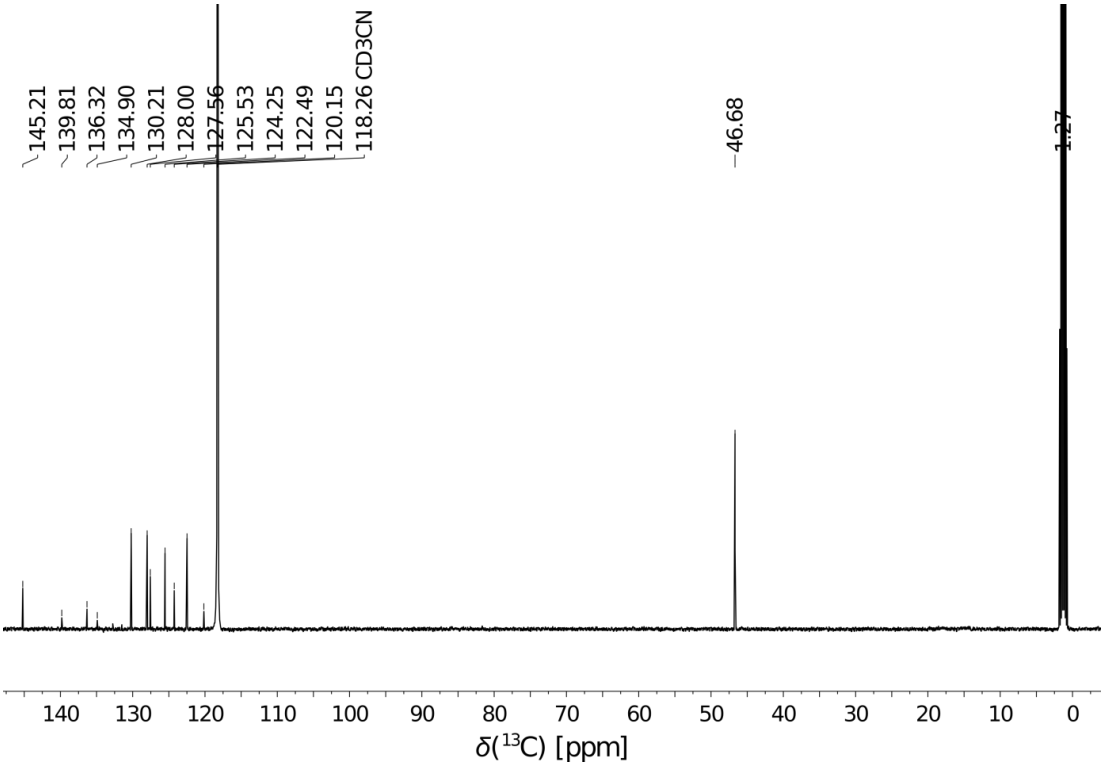


Figure S29. Full $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, CD_3CN) of [**1**-SH][**3**-H].

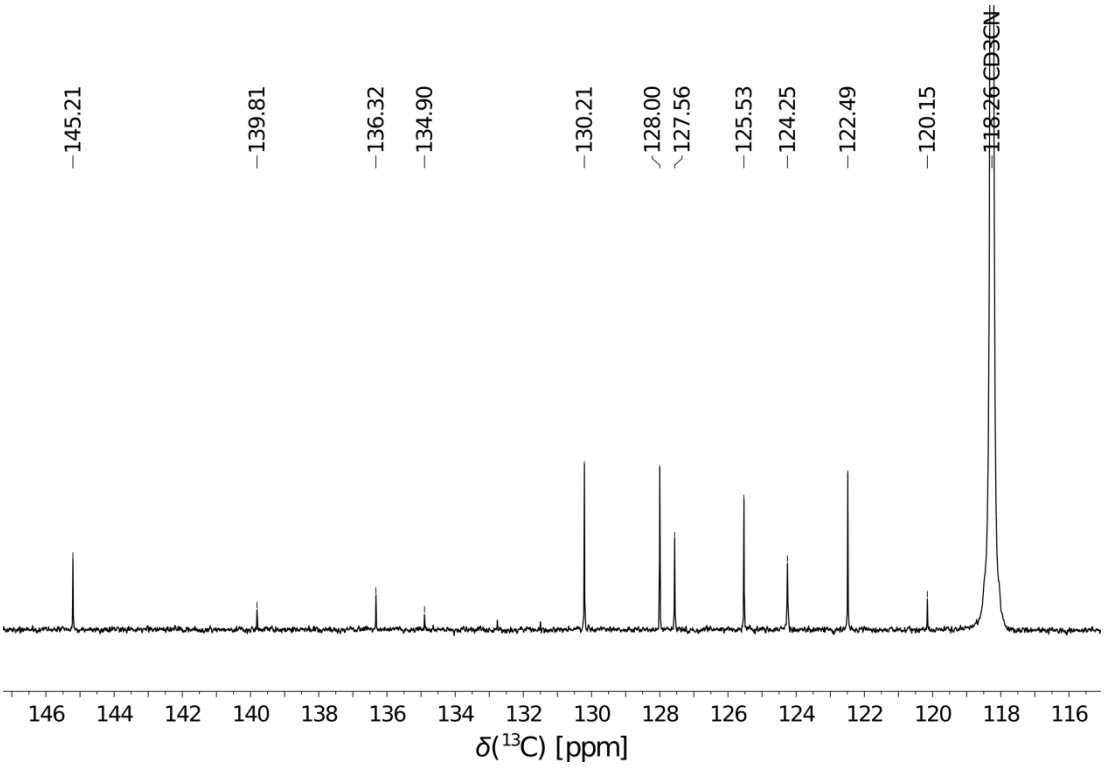


Figure S30. Excerpt of the $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, CD_3CN) of [**1**-SH][**3**-H].

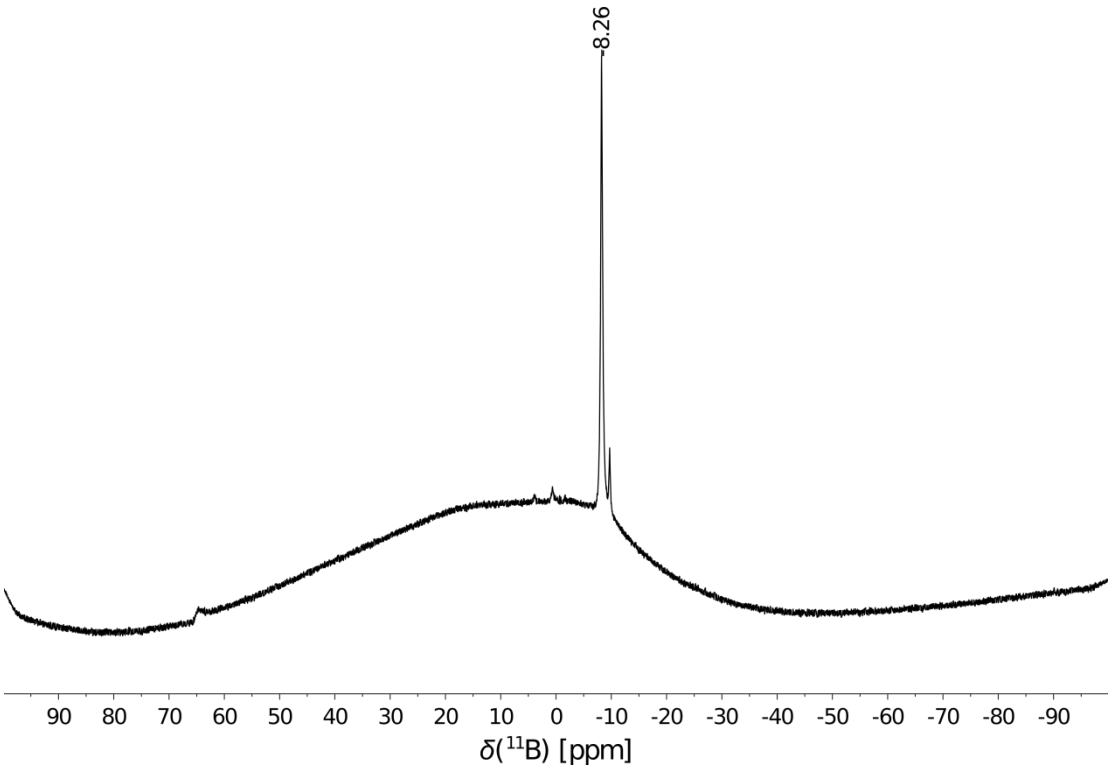


Figure S31. ^{11}B NMR spectrum (160 MHz, CD_3CN) of [**1**-SH][**3**-H].

[1-PH$_2$][3-H]

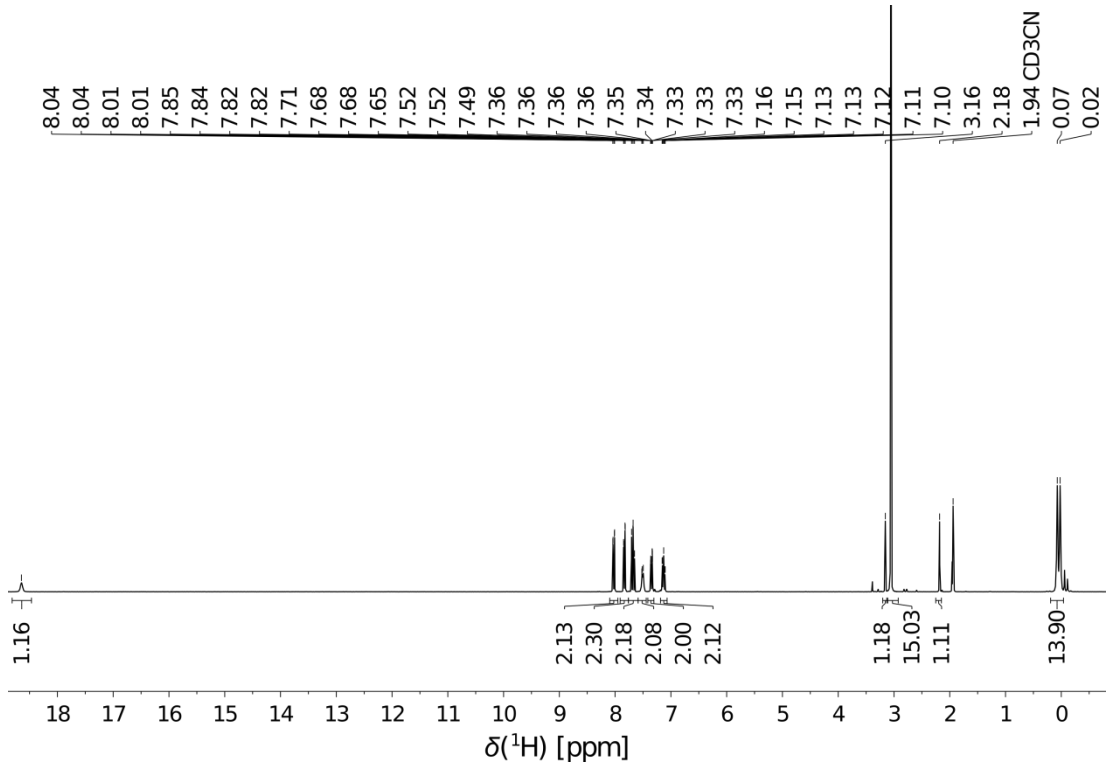


Figure S32. Full ^1H NMR spectrum (300 MHz, CD_3CN) of [**1**-PH$_2$][**3**-H].

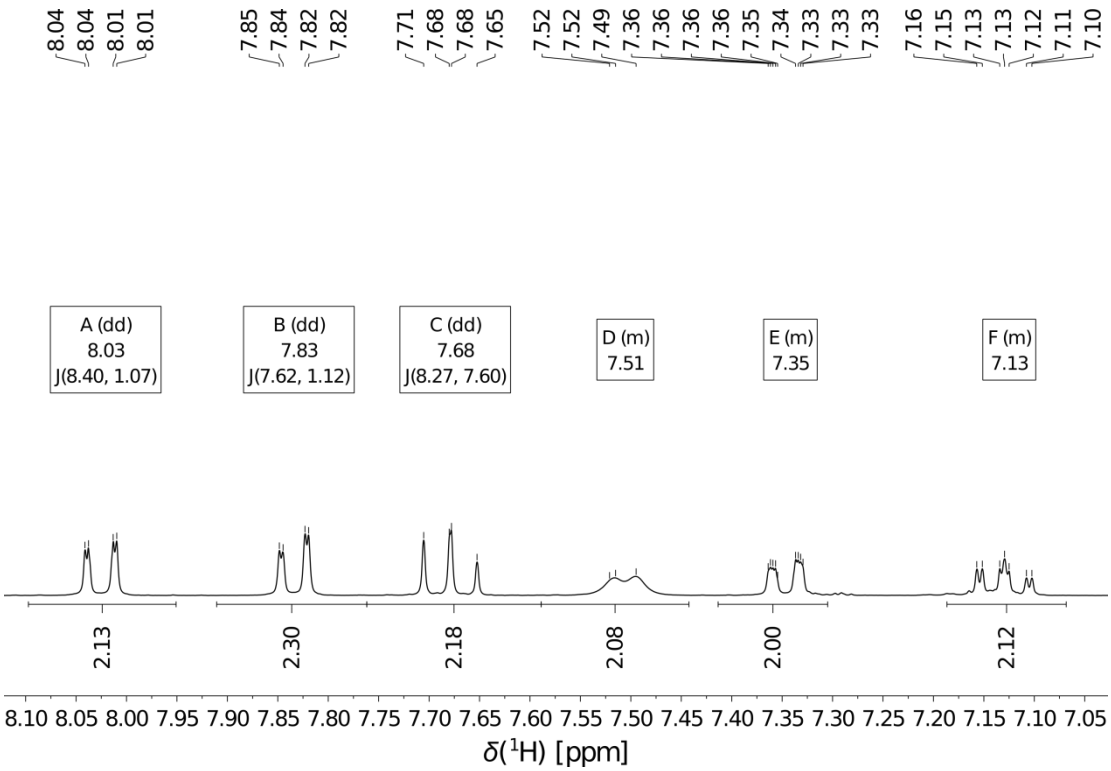


Figure S33. Excerpt of the ^{1}H NMR spectrum (300 MHz, CD_3CN) of [**1**-PH_2][**3**-H] containing the signals of protons bound to the naphthalene backbones.

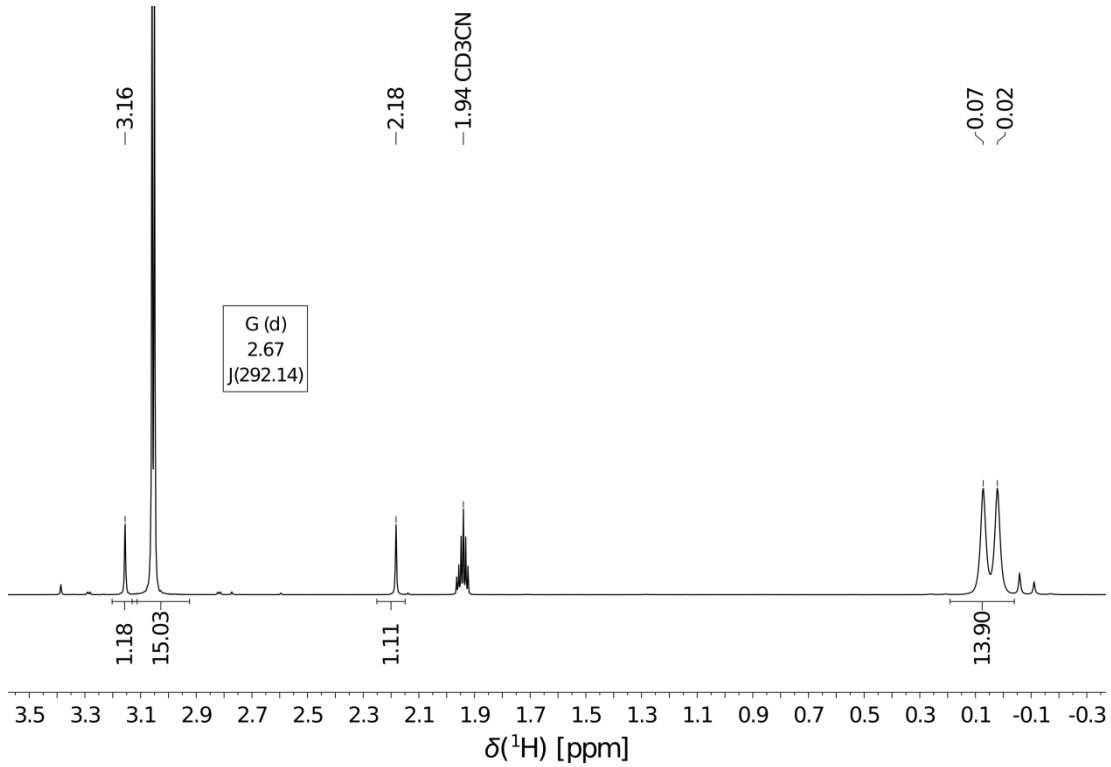


Figure S34. Excerpt of the ^{1}H NMR spectrum (300 MHz, CD_3CN) of [**1**-PH_2][**3**-H] containing the signals of the protons of the methyl groups as well as P*H*$_2$.

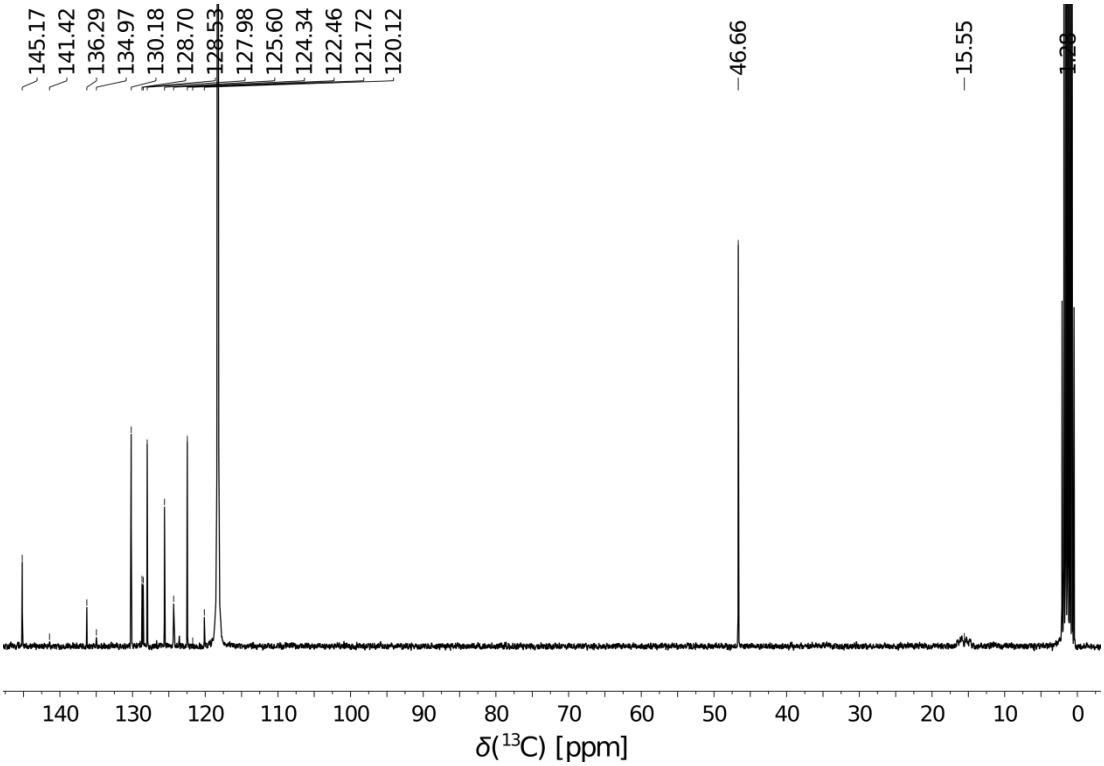


Figure S35. Full $^{13}C\{^{1}H\}$ NMR spectrum (75 MHz, CD_3CN) of [**1**-PH_2][**3**-H].

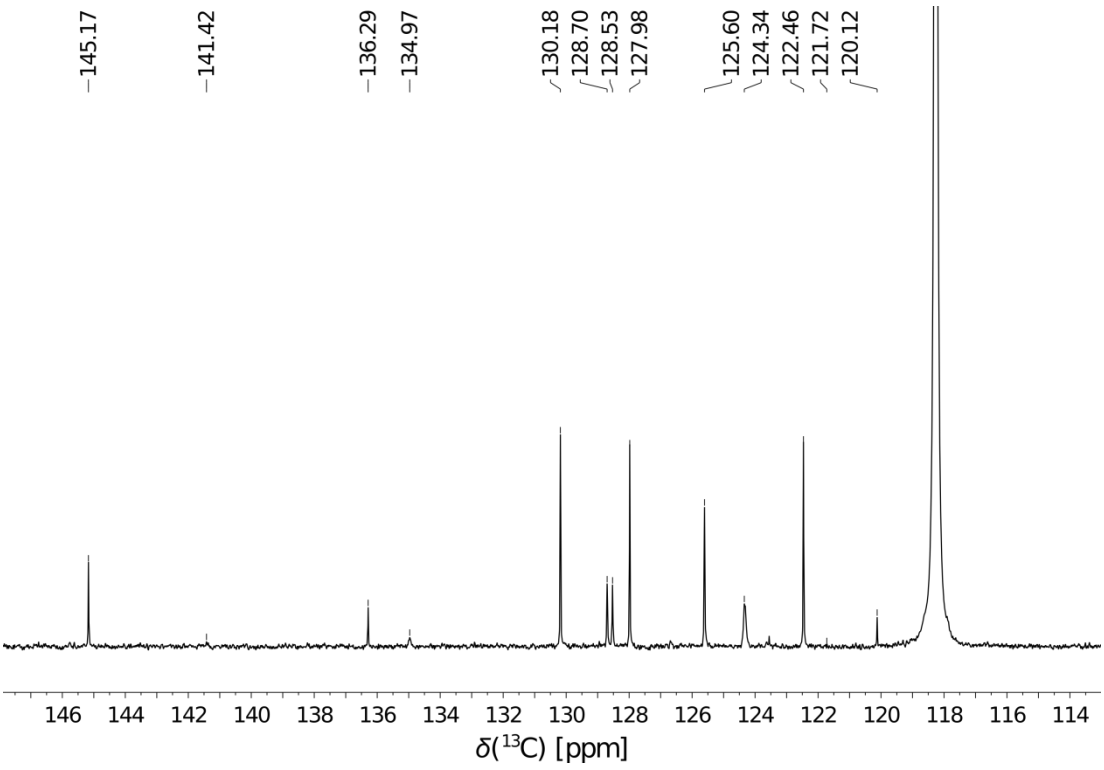


Figure S36. Excerpt of the $^{13}C\{^{1}H\}$ NMR spectrum (75 MHz, CD_3CN) of [**1**-PH_2][**3**-H].

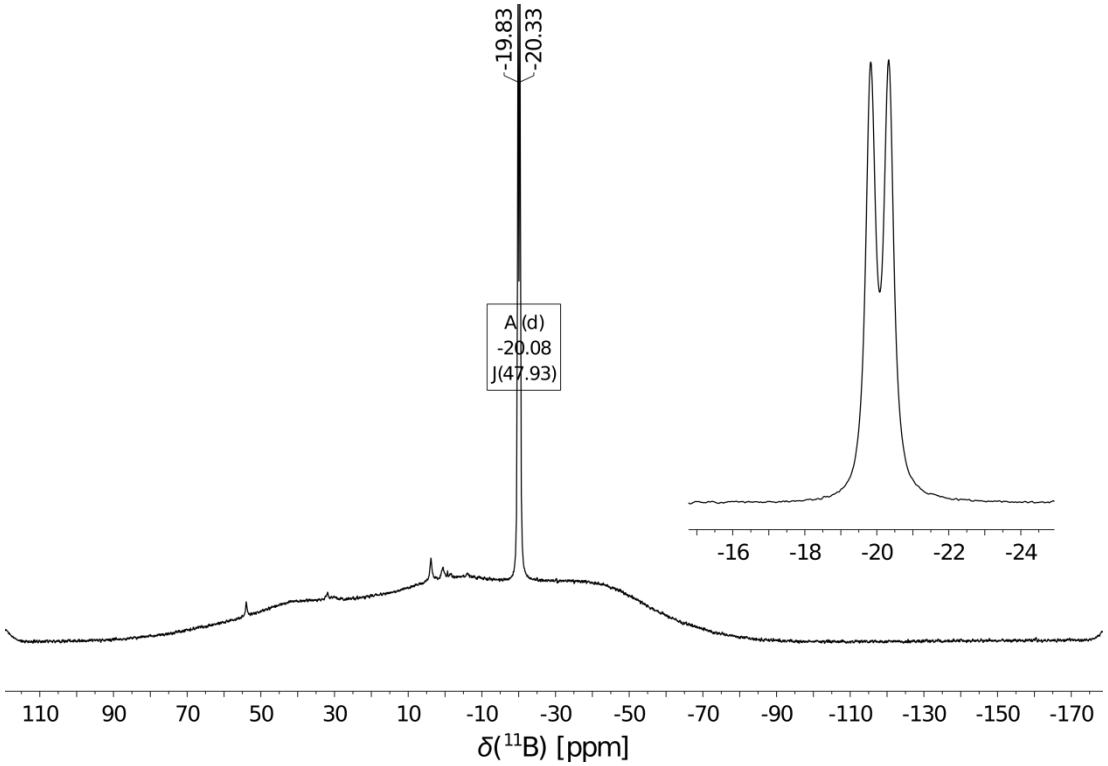


Figure S37. ^{11}B NMR spectrum (96 MHz, CD_3CN) of [**1**-PH_2][**3**-H].

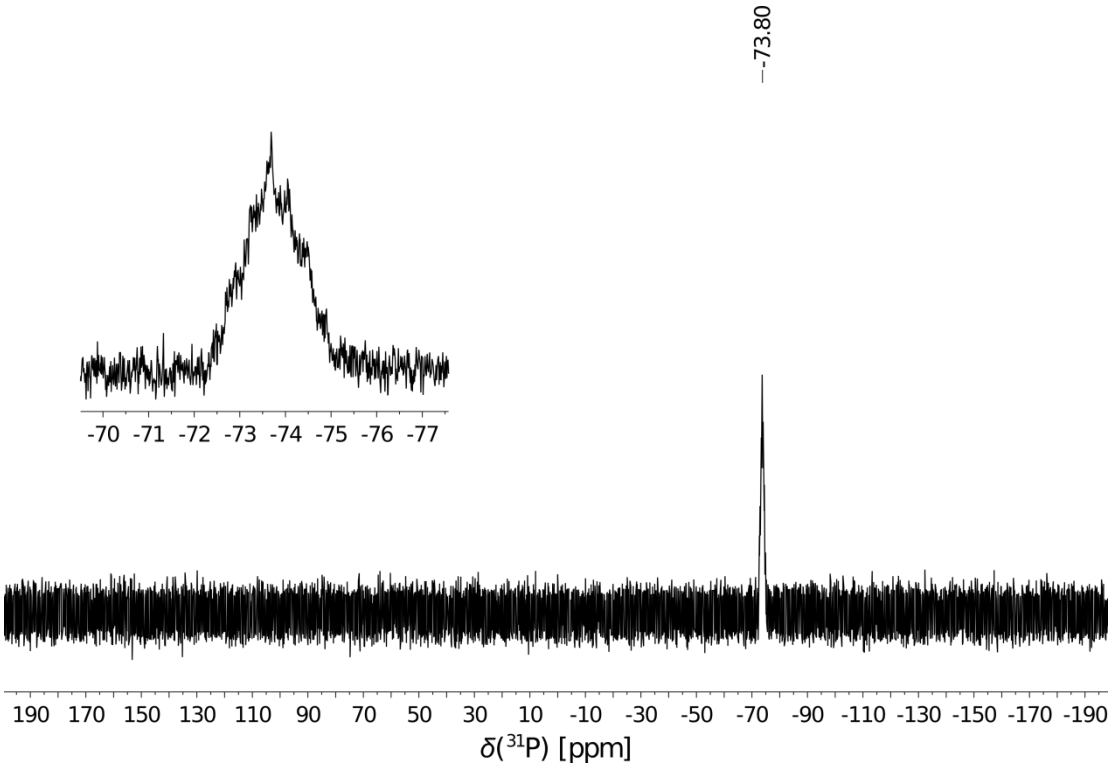


Figure S38. $^{31}P\{^1H\}$ NMR spectrum (121 MHz, CD_3CN) of [**1**-PH_2][**3**-H].

[1-SeH][3-H]

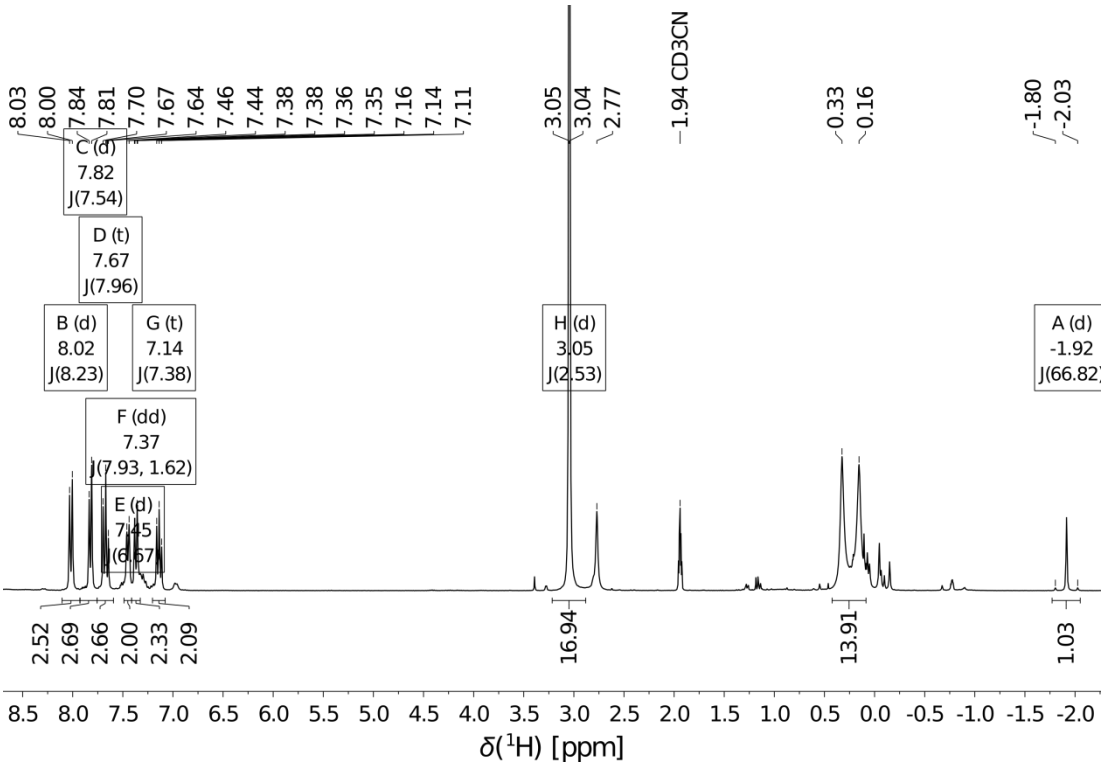


Figure S39. Full ^{1}H NMR spectrum (300 MHz, CD_3CN) of [**1**-SeH][**3**-H].

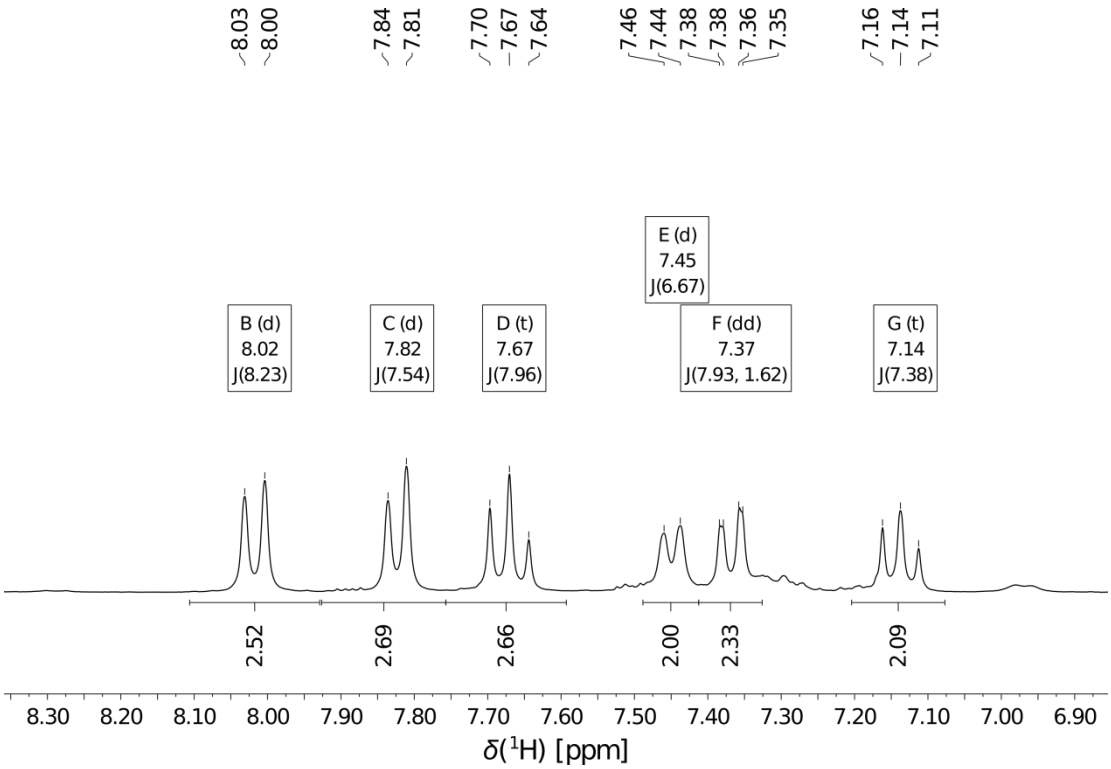


Figure S40. Excerpt of the ^{1}H NMR spectrum (300 MHz, CD_3CN) of [**1**-SeH][**3**-H] containing the signals of protons bound to the naphthalene backbones.

[1-CN][3-H]

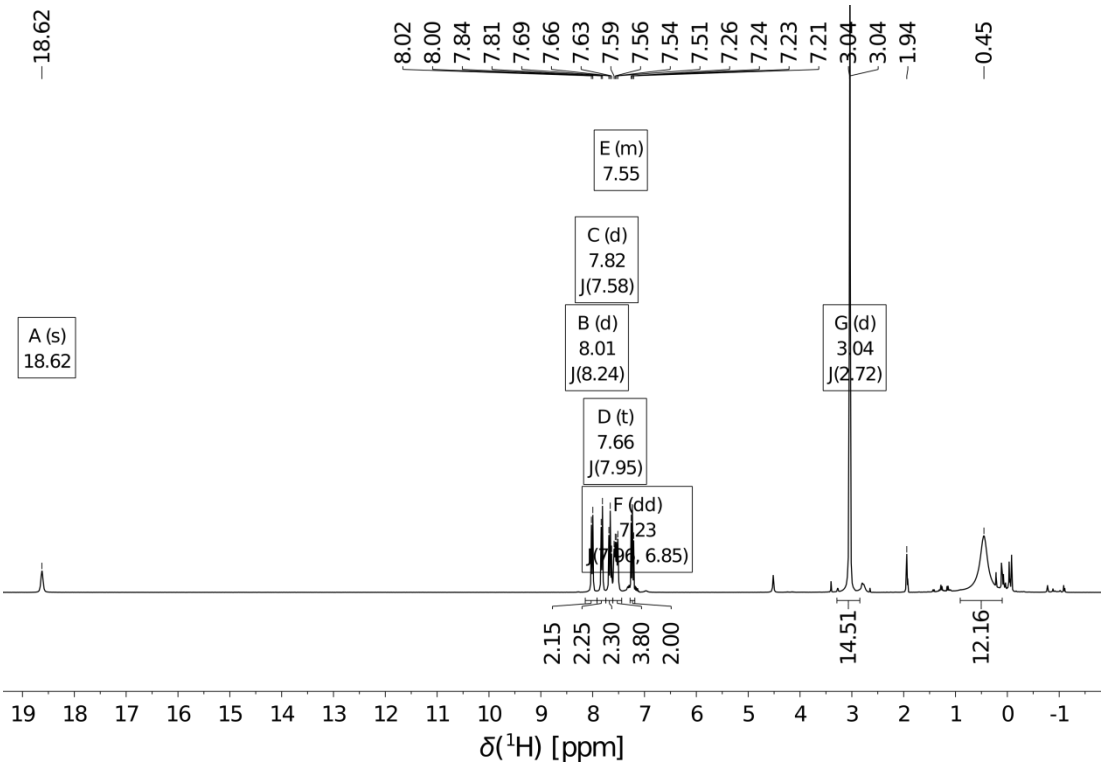


Figure S41. Full ^{1}H NMR spectrum (300 MHz, CD_3CN) of [**1**-CN][**3**-H].

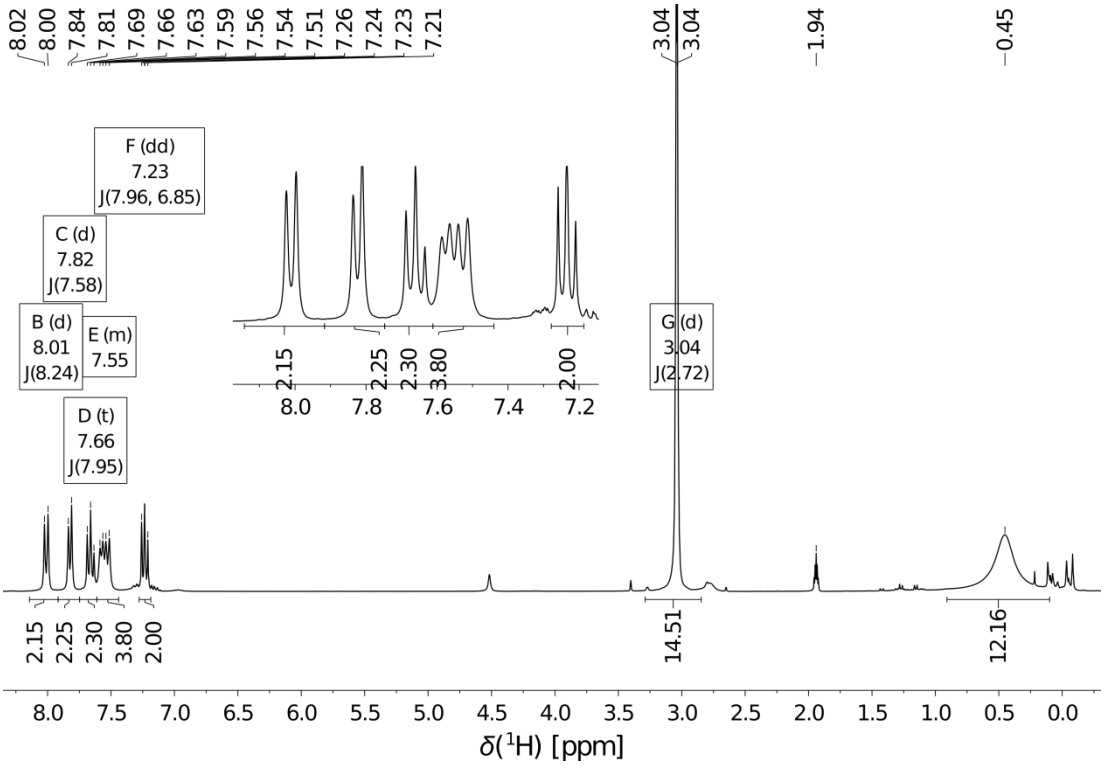


Figure S42. Excerpt of the ^{1}H NMR spectrum (300 MHz, CD_3CN) of [**1**-CN][**3**-H].

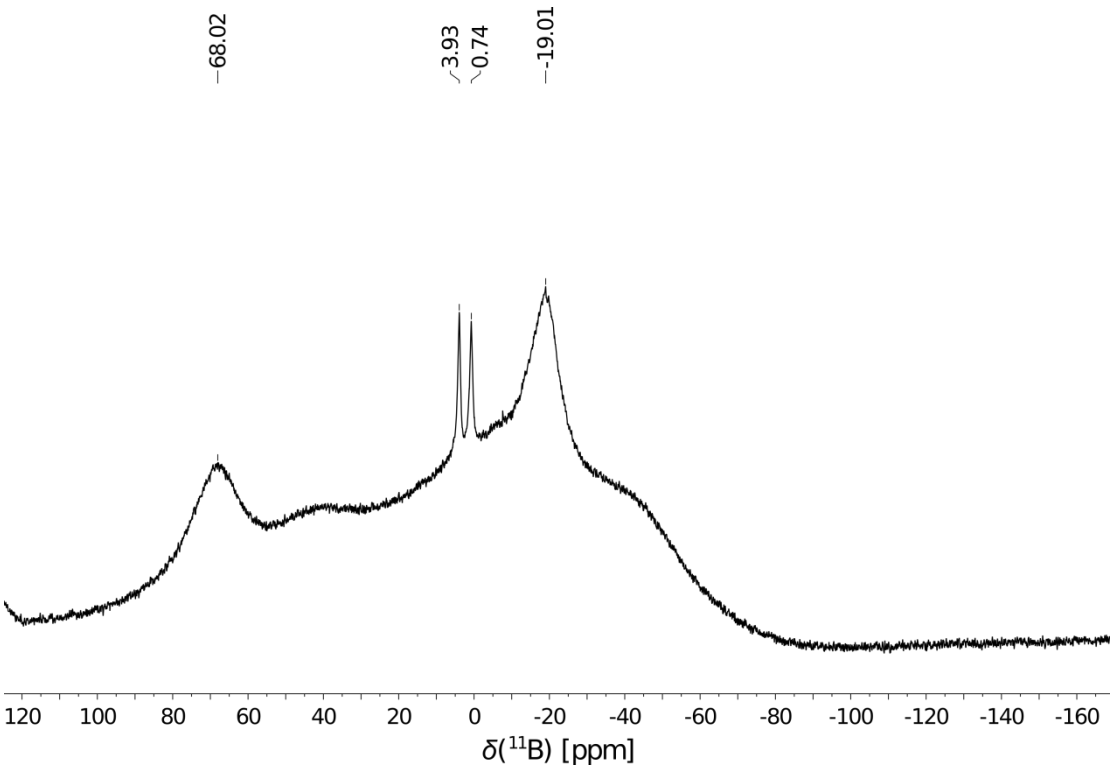


Figure S43. ^{11}B NMR spectrum (96 MHz, CD_3CN) of [**1**-NH_2][**3**-H].

1,2-Bis(trimethylsilyl)benzene

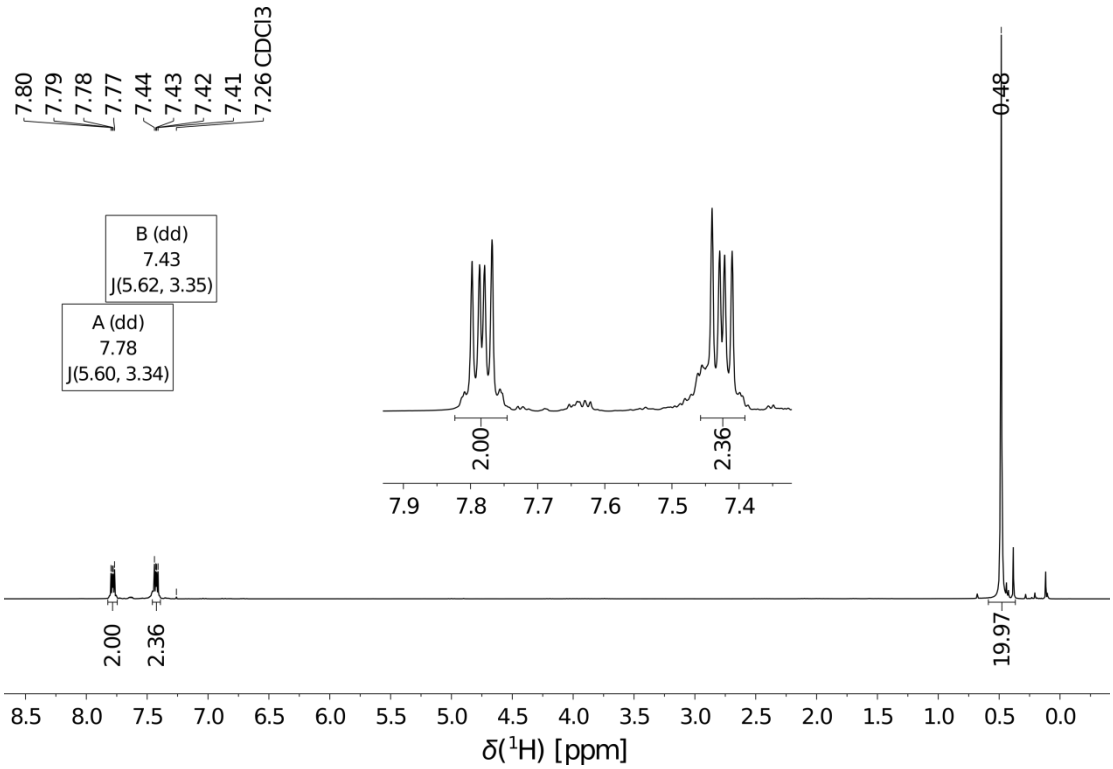


Figure S44. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 1,2-bis(trimethylsilyl)benzene.

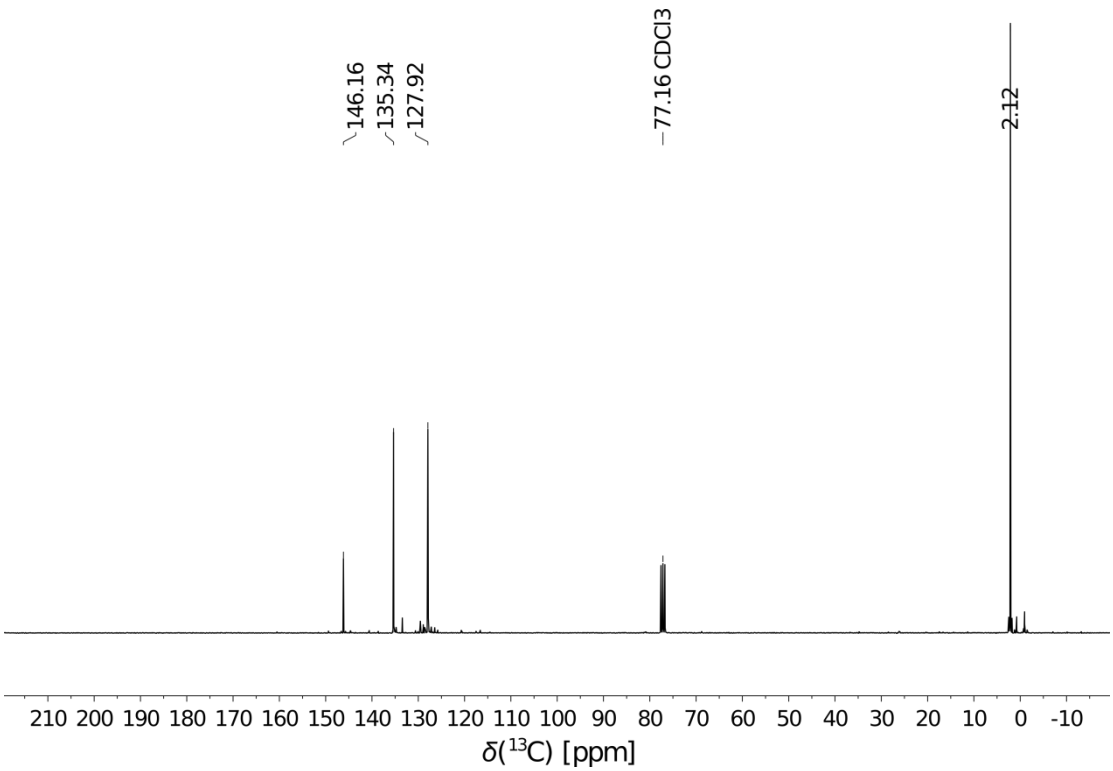


Figure S45. $^{13}C\{^{1}H\}$ NMR spectrum (75 MHz, $CDCl_3$) of 1,2-bis(trimethylsilyl)benzene.

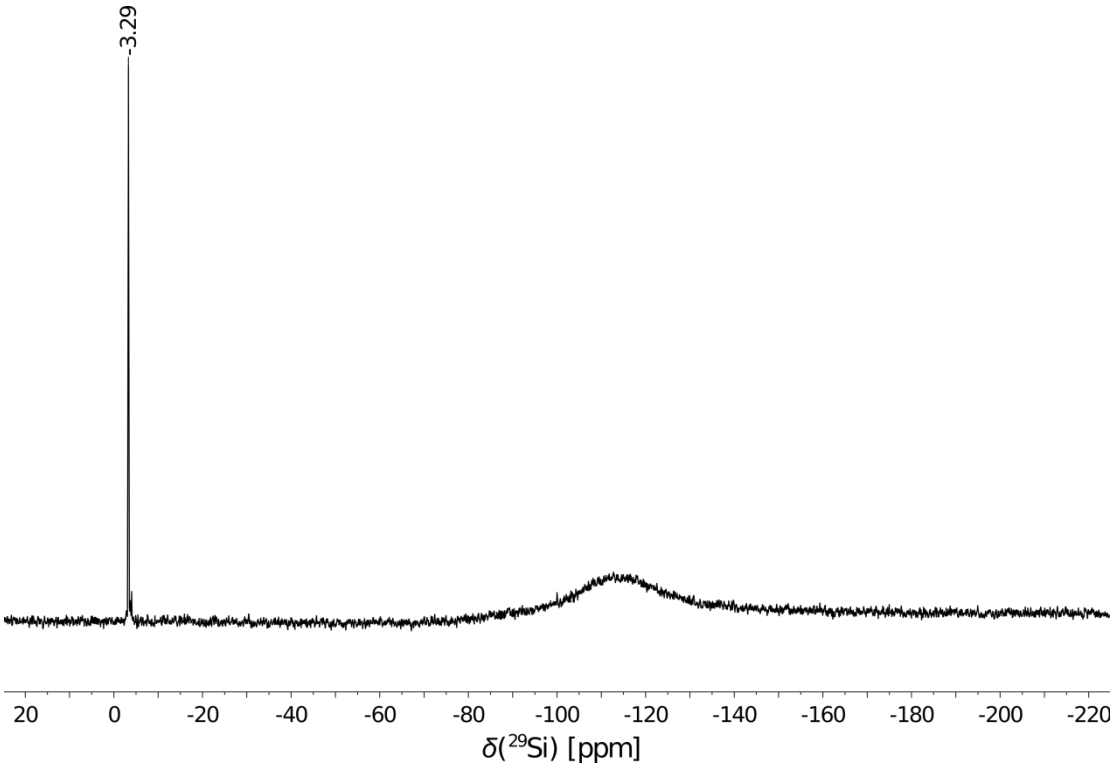


Figure S46. $^{29}Si\{^{1}H\}$ NMR spectrum (60 MHz, $CDCl_3$) of 1,2-bis(trimethylsilyl)benzene.

1,2-Bis(dichloroboryl)benzene

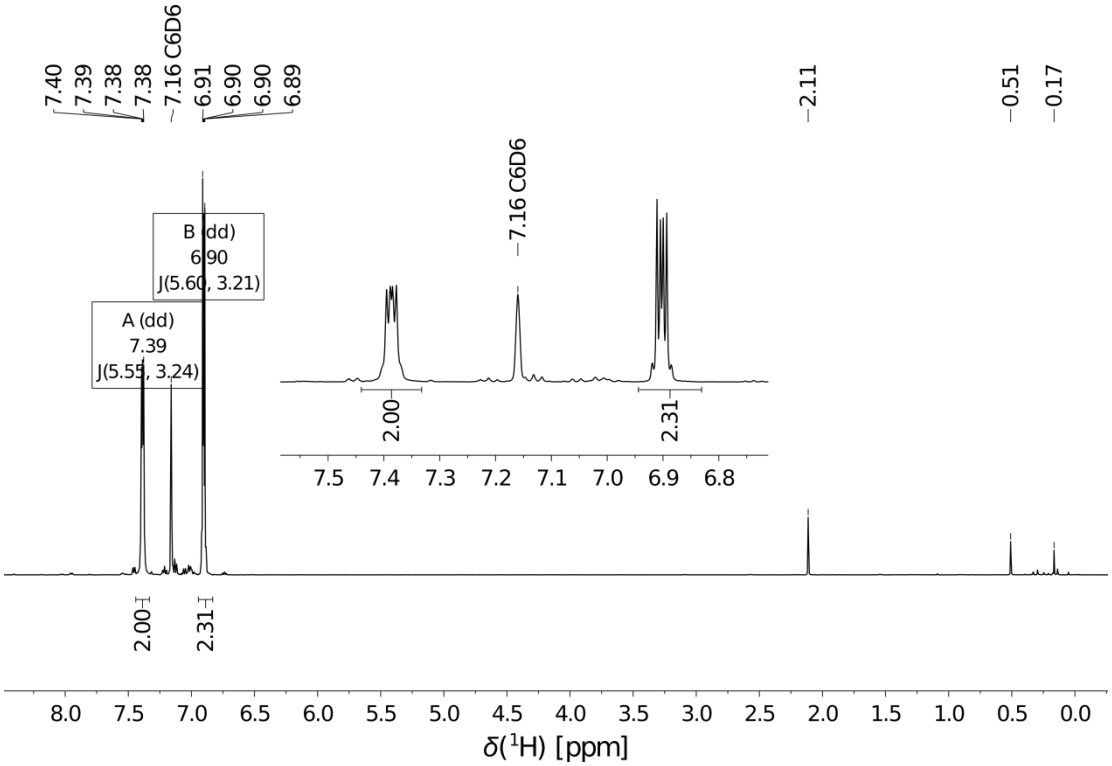


Figure S47. ^{1}H NMR spectrum (300 MHz, C_6D_6) of 1,2-bis(dichoroboryl)benzene.

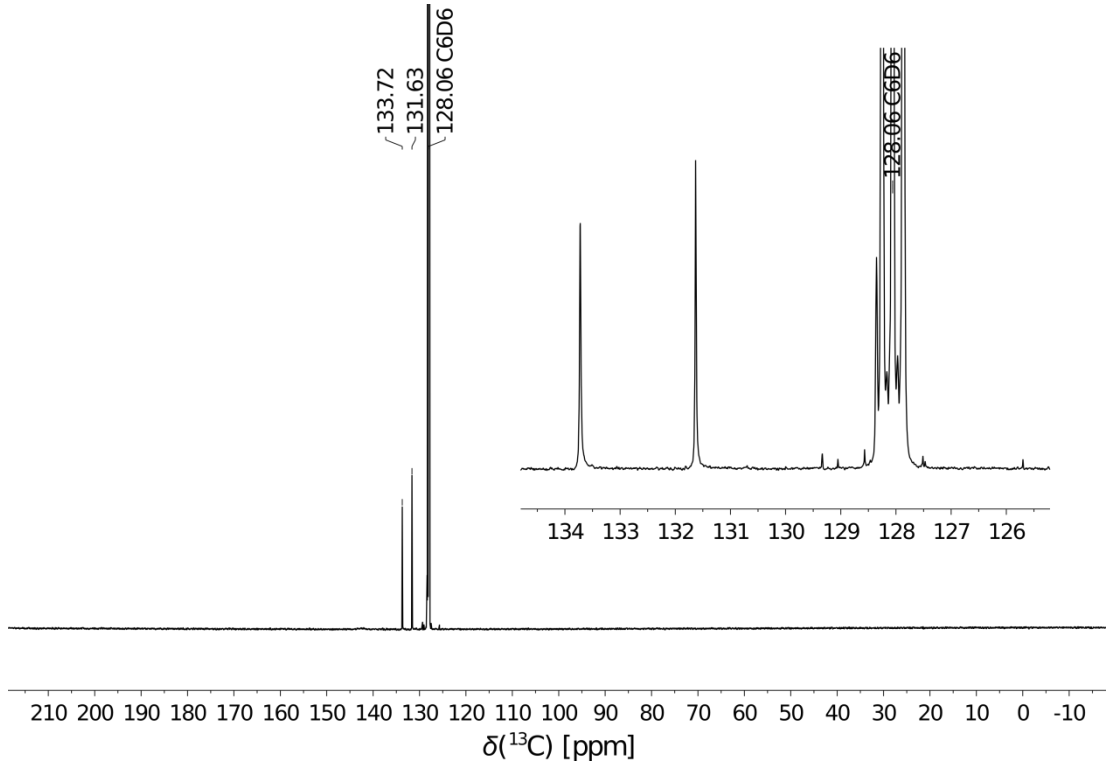


Figure S48. $^{13}C\{^{1}H\}$ NMR spectrum (75 MHz, C_6D_6) of 1,2-bis(dichloroboryl)benzene.

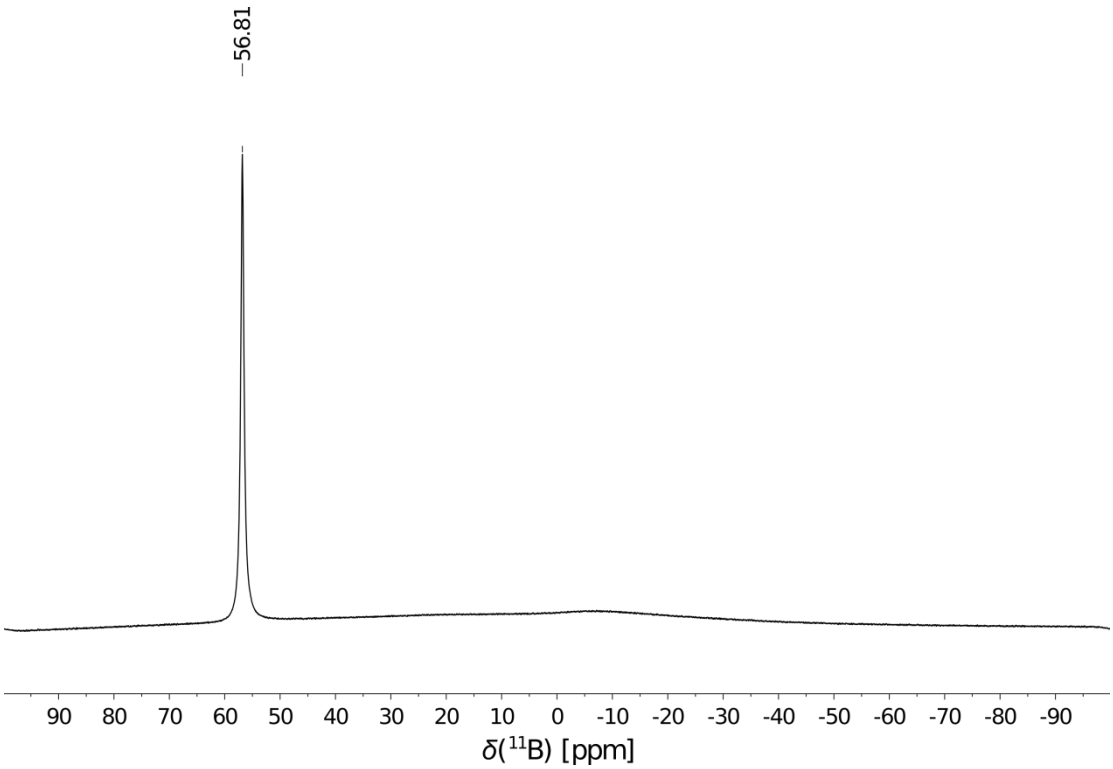


Figure S49. ^{11}B NMR spectrum (96 MHz, C_6D_6) of 1,2-bis(dichloroboryl)benzene.

1,2-Bis(dimethylboryl)benzene

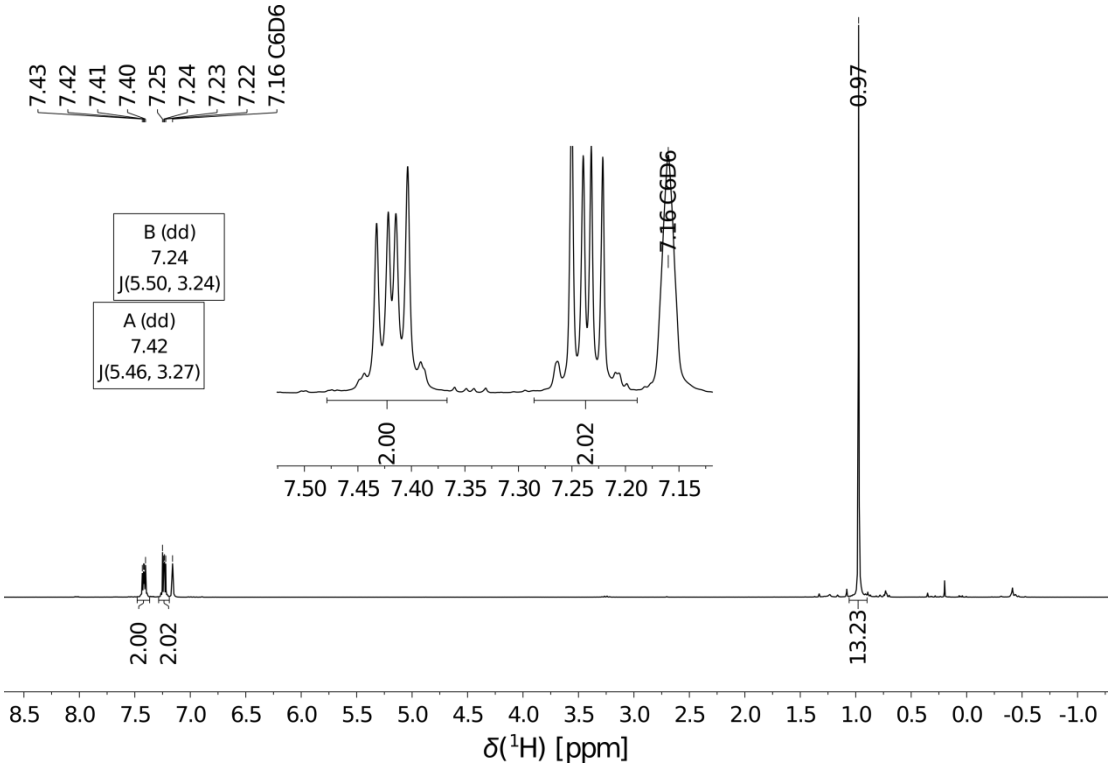


Figure S50. ^{1}H NMR spectrum (300 MHz, C_6D_6) of 1,2-bis(dimethylboryl)benzene.

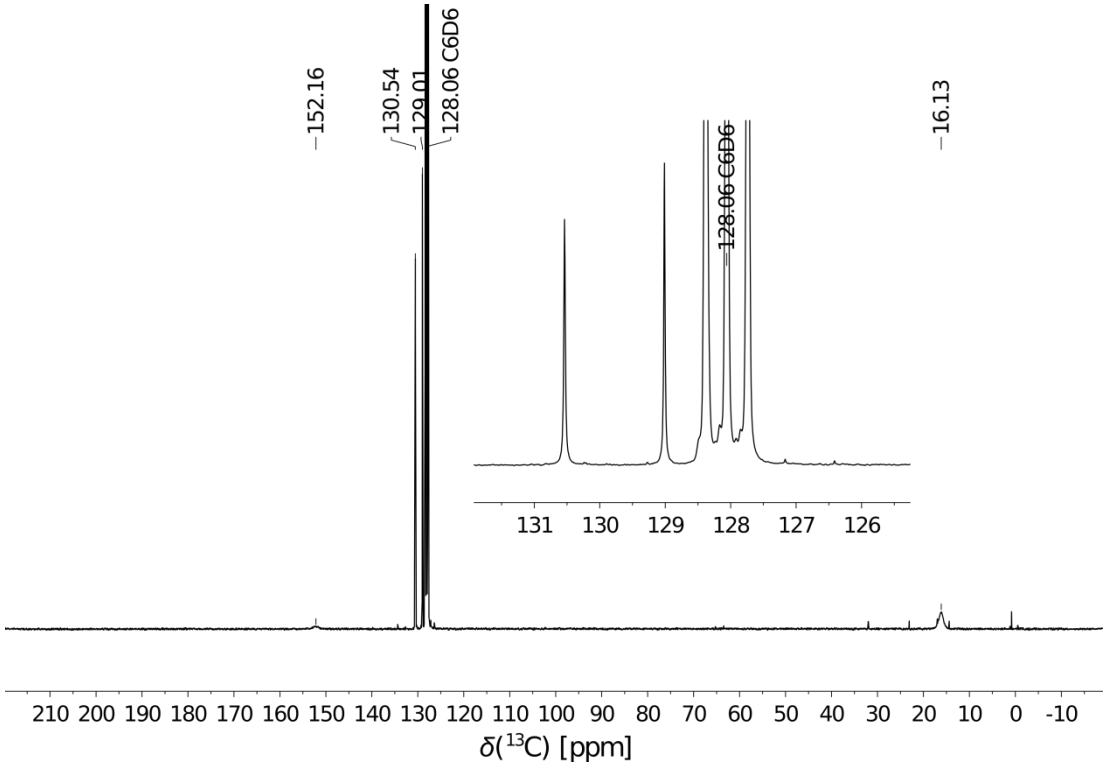


Figure S51. $^{13}C\{^{1}H\}$ NMR spectrum (75 MHz, C_6D_6) of 1,2-bis(dimethylboryl)benzene.

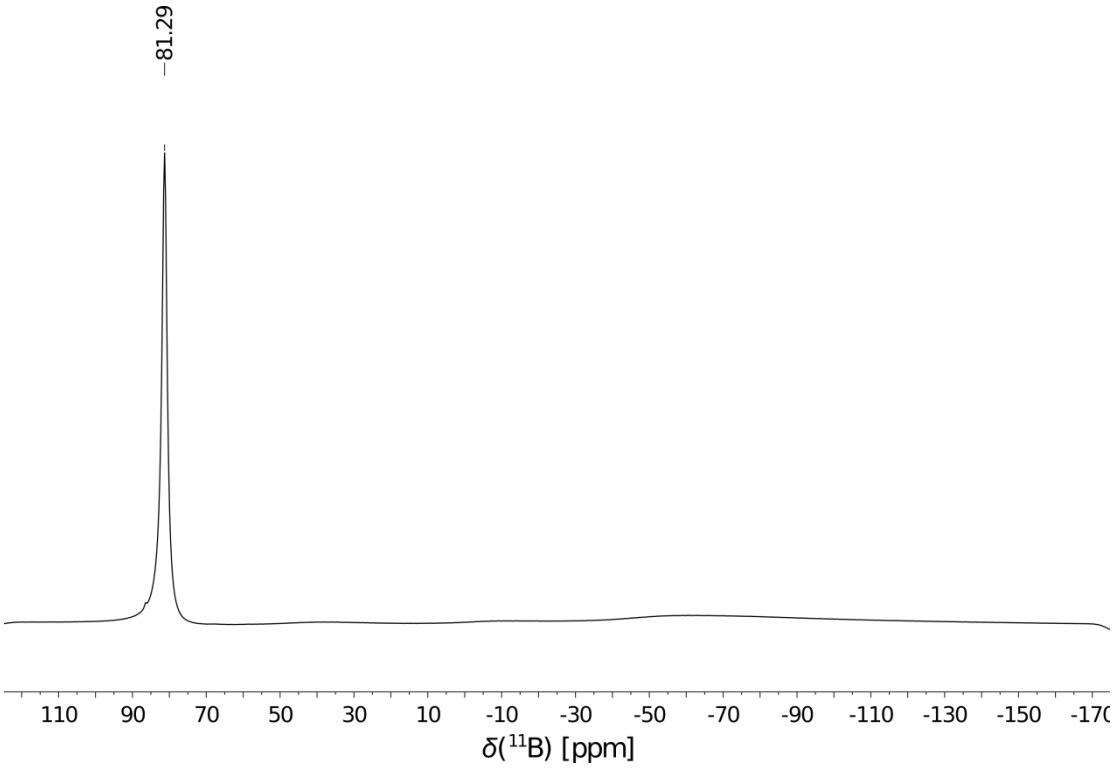


Figure S52. ^{11}B NMR spectrum (96 MHz, C_6D_6) of 1,2-bis(dimethylboryl)benzene.

[2-PH$_2$][3-H]

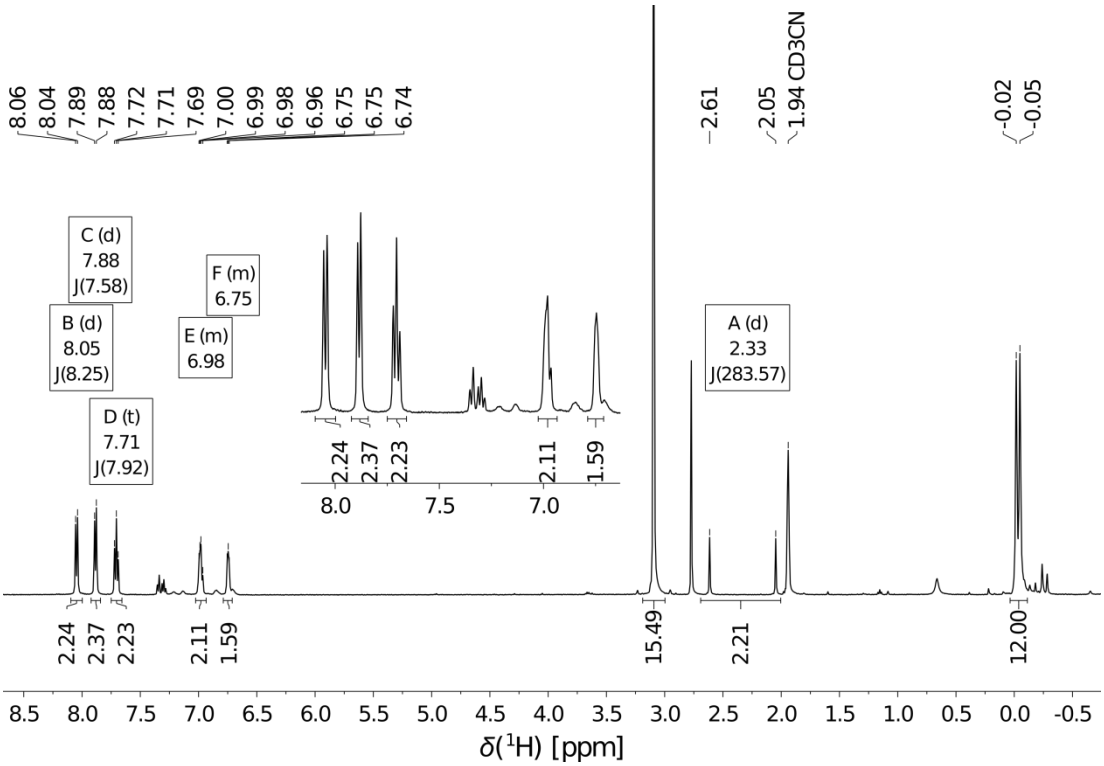


Figure S53. ^{1}H NMR spectrum (500 MHz, CD_3CN) of [**2**-PH_2][**3**-H].

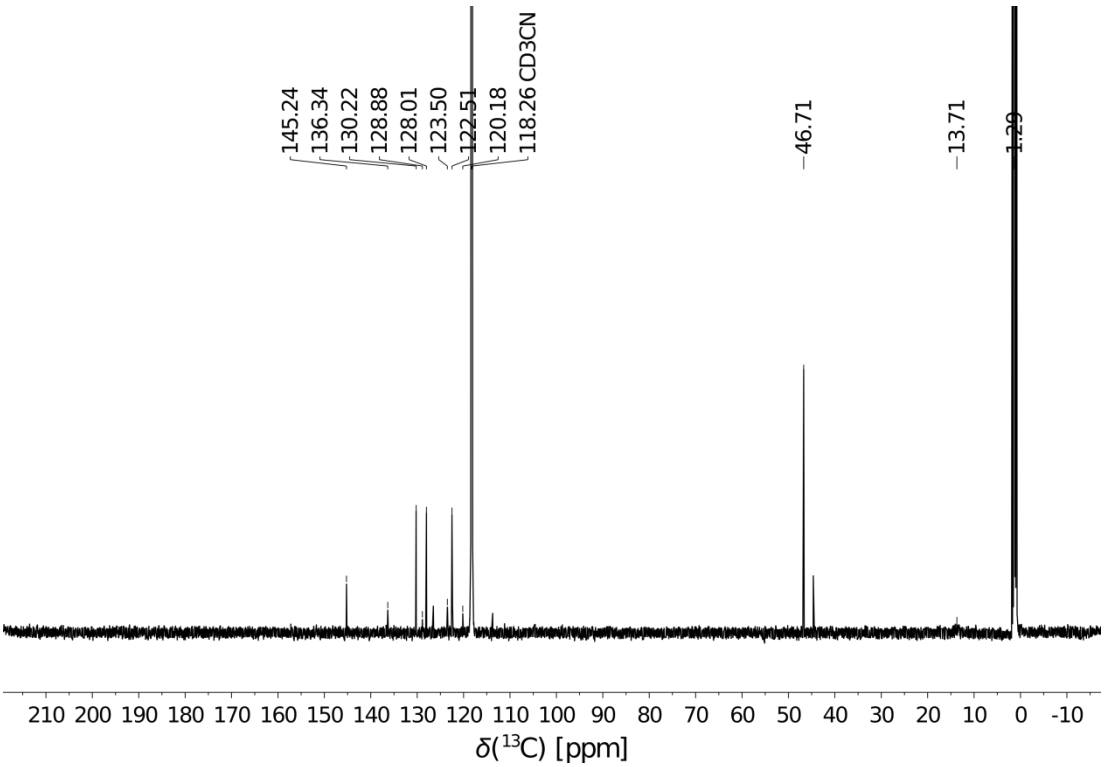


Figure S54. Full $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, CD_3CN) of [**2**-PH_2][**3**-H].

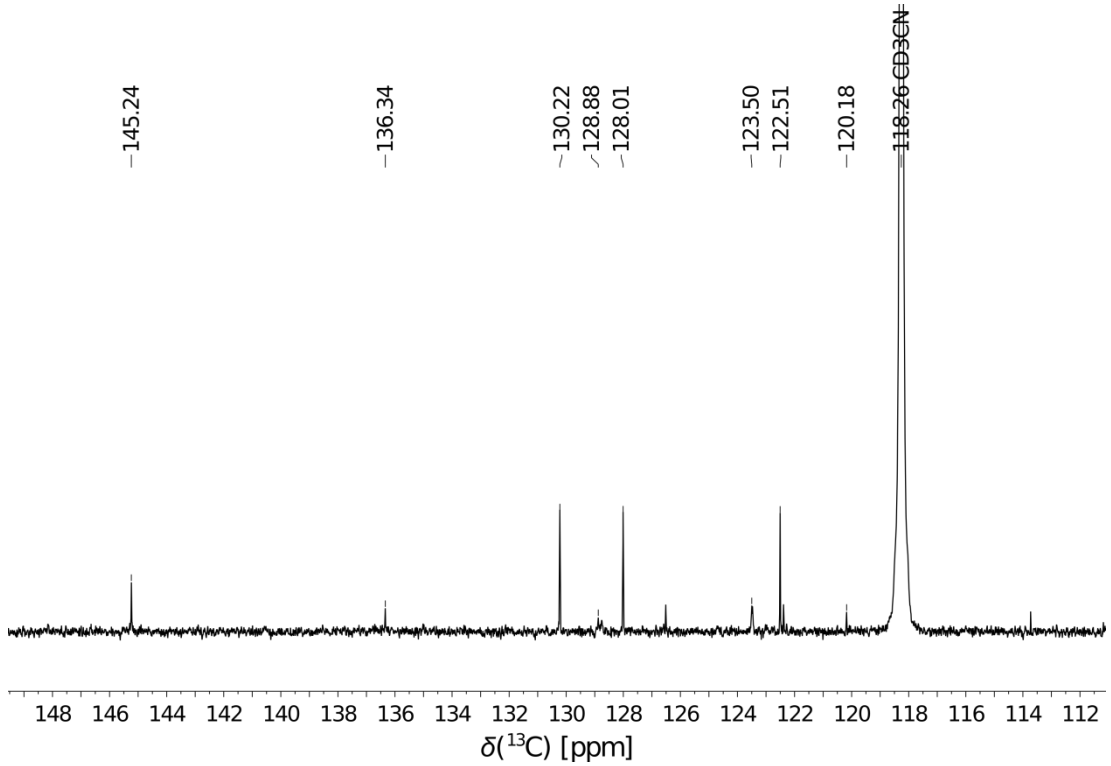


Figure S55. Excerpt of the $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, CD_3CN) of [**2**-PH_2][**3**-H].

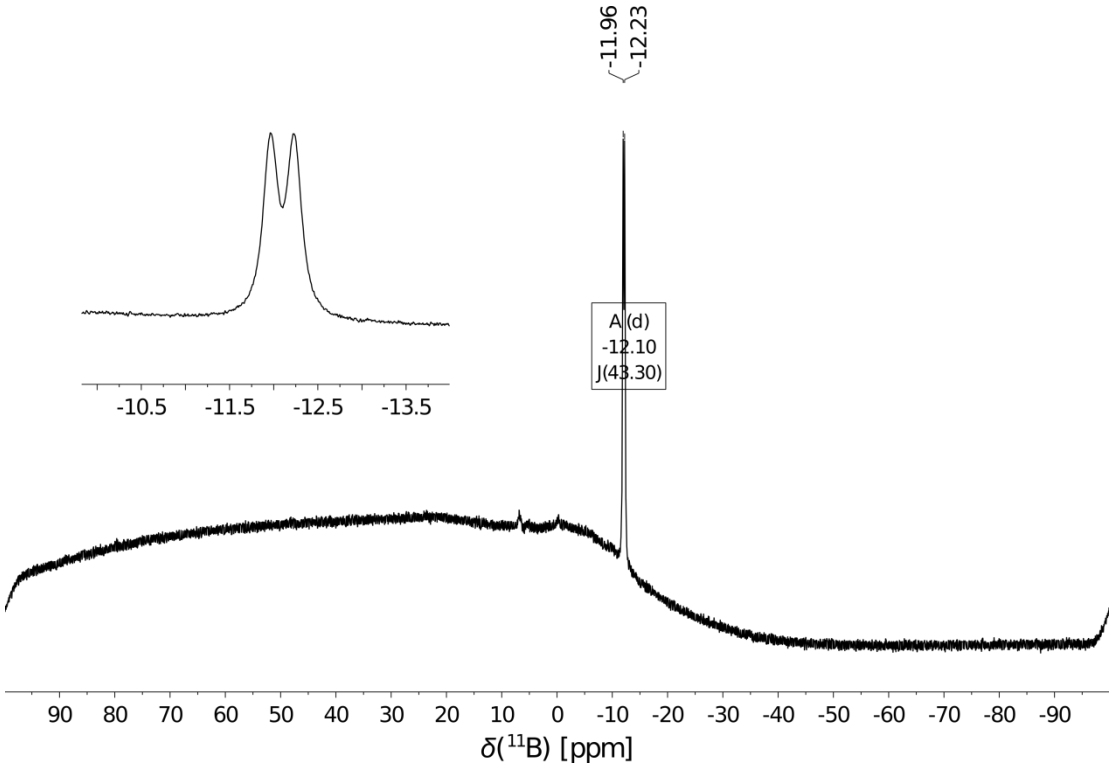


Figure S56. ^{11}B NMR spectrum (160 MHz, CD_3CN) of [**2**-PH_2][**3**-H].

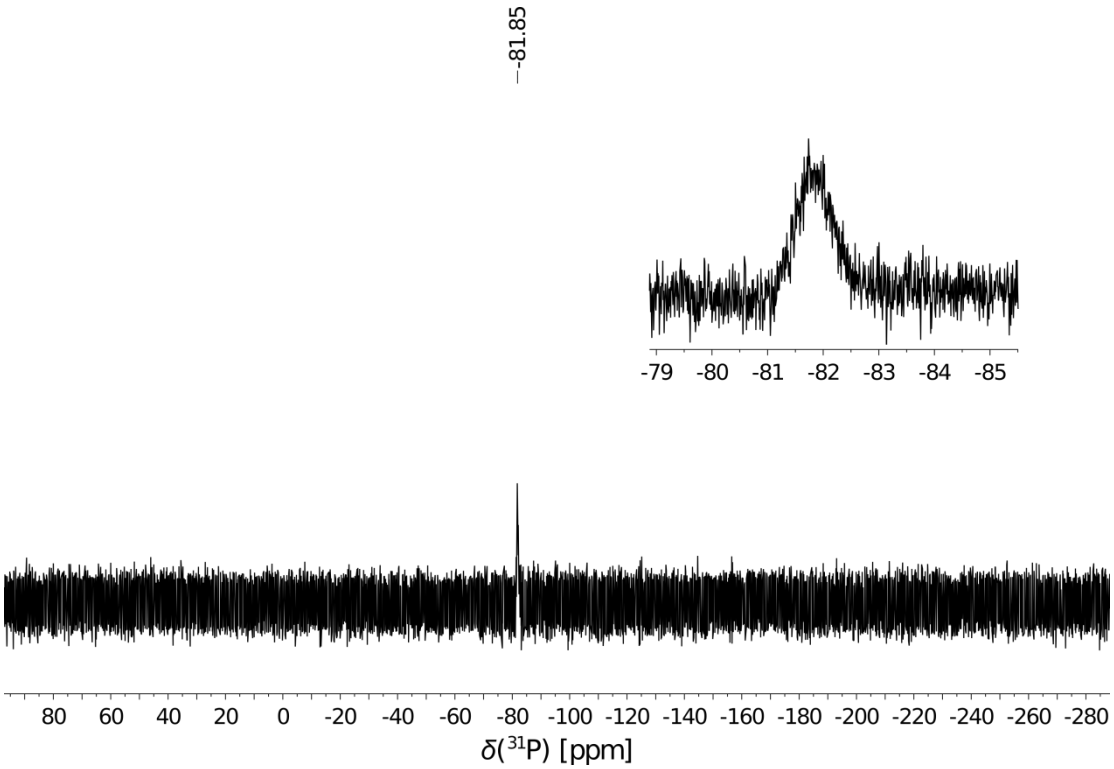


Figure S57. $^{31}P\{^{1}H\}$ NMR spectrum (202 MHz, CD_3CN) of [**1**-PH_2][**3**-H].

[3-H]Cl

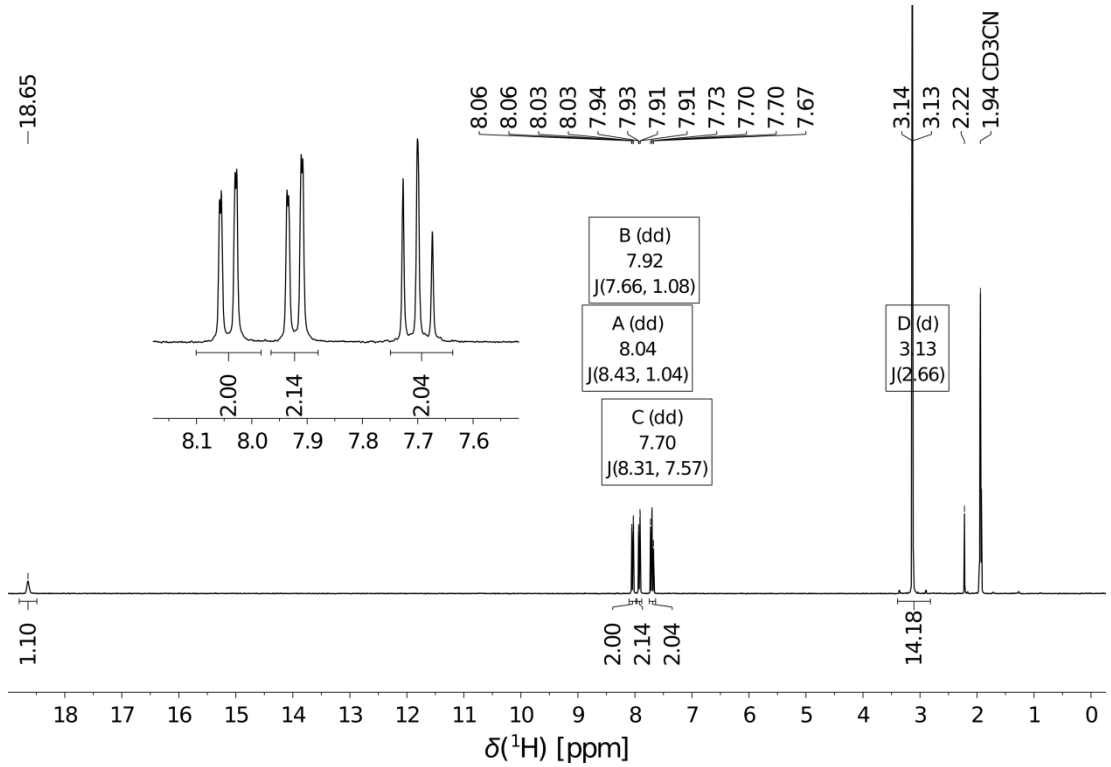


Figure S58. ^{1}H NMR spectrum (300 MHz, CD_3CN) of [**3**-H]Cl.

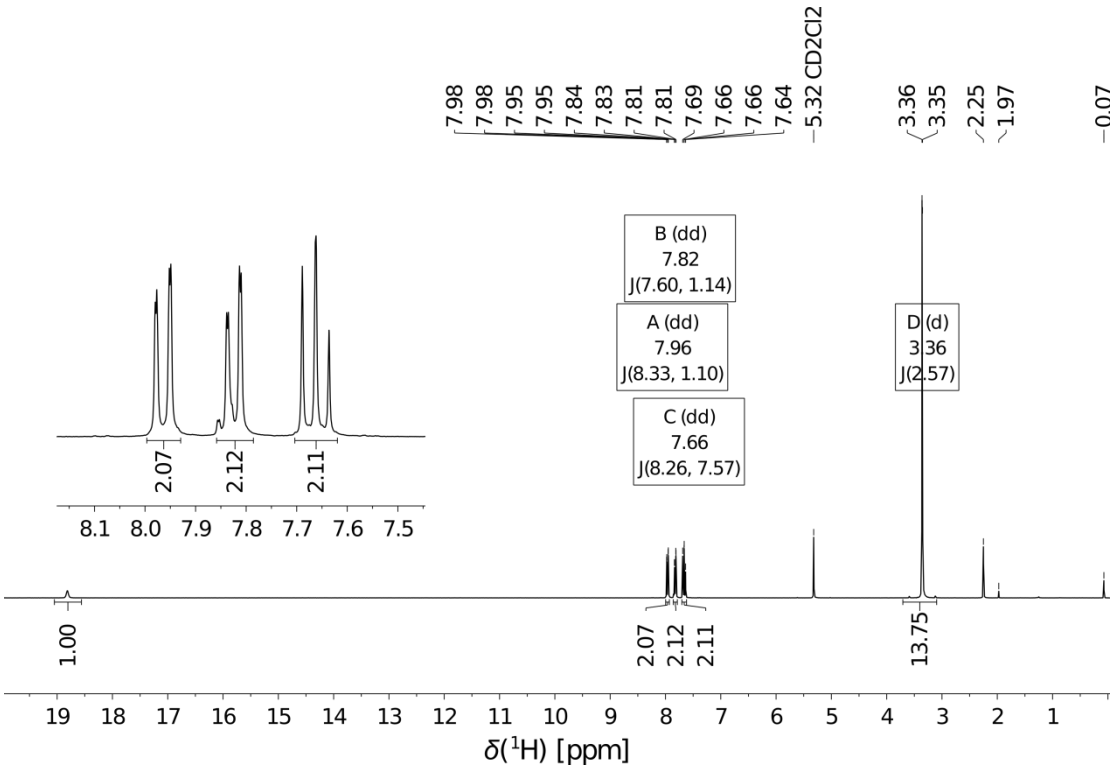


Figure S59. ^{1}H NMR spectrum (300 MHz, CD_2Cl_2) of [**3**-H]Cl.

[1-H][3-H]

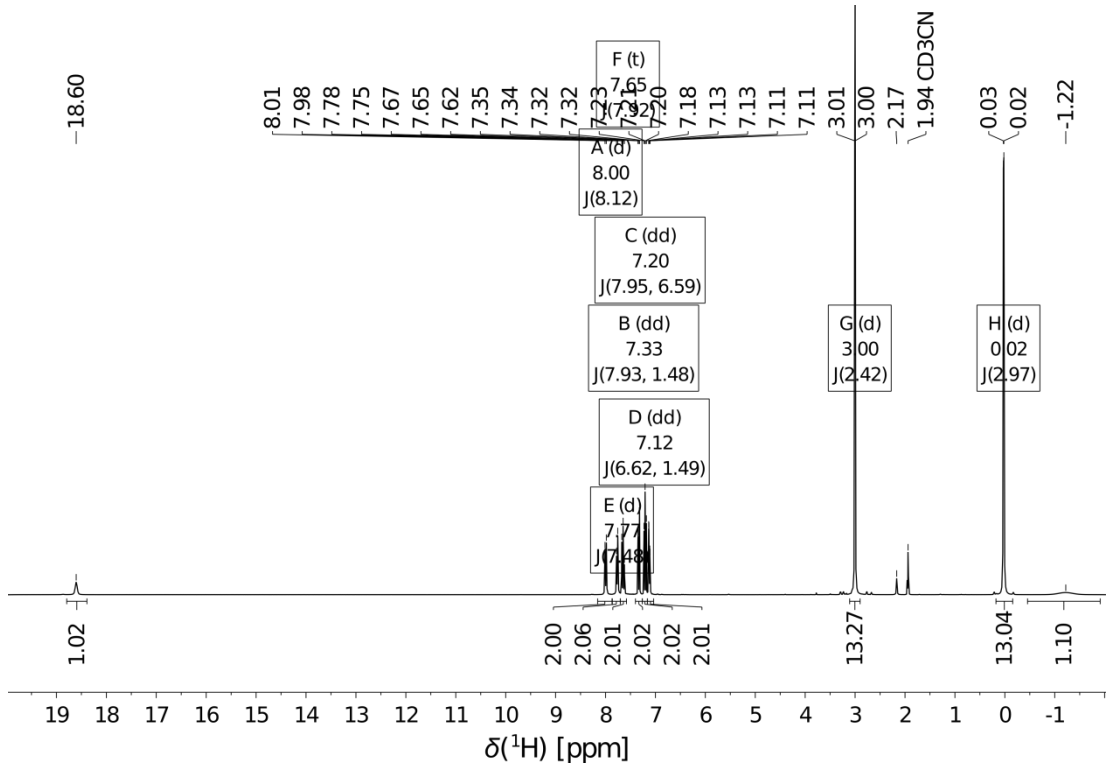


Figure S60. Full ^{1}H NMR spectrum (300 MHz, CD_3CN) of [**1**-H][**3**-H].

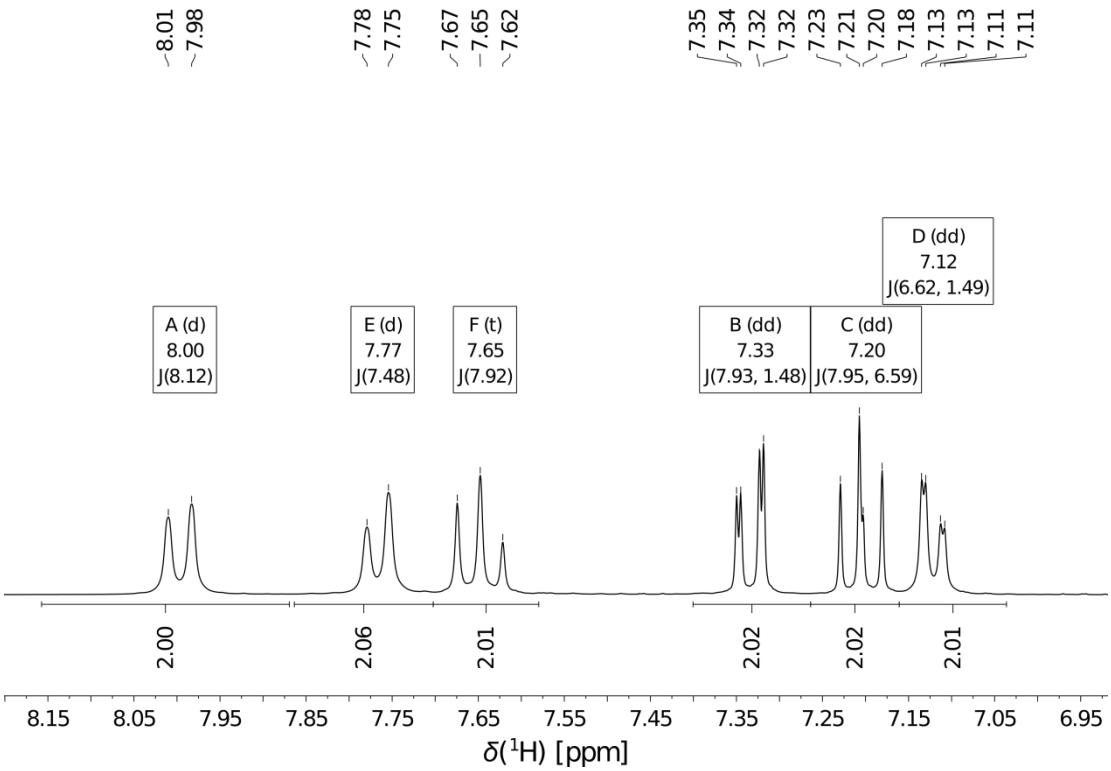


Figure S61. Excerpt of the ^{1}H NMR spectrum (300 MHz, CD_3CN) of [**1**-H][**3**-H] containing the signals of protons bound to the naphthalene backbones.

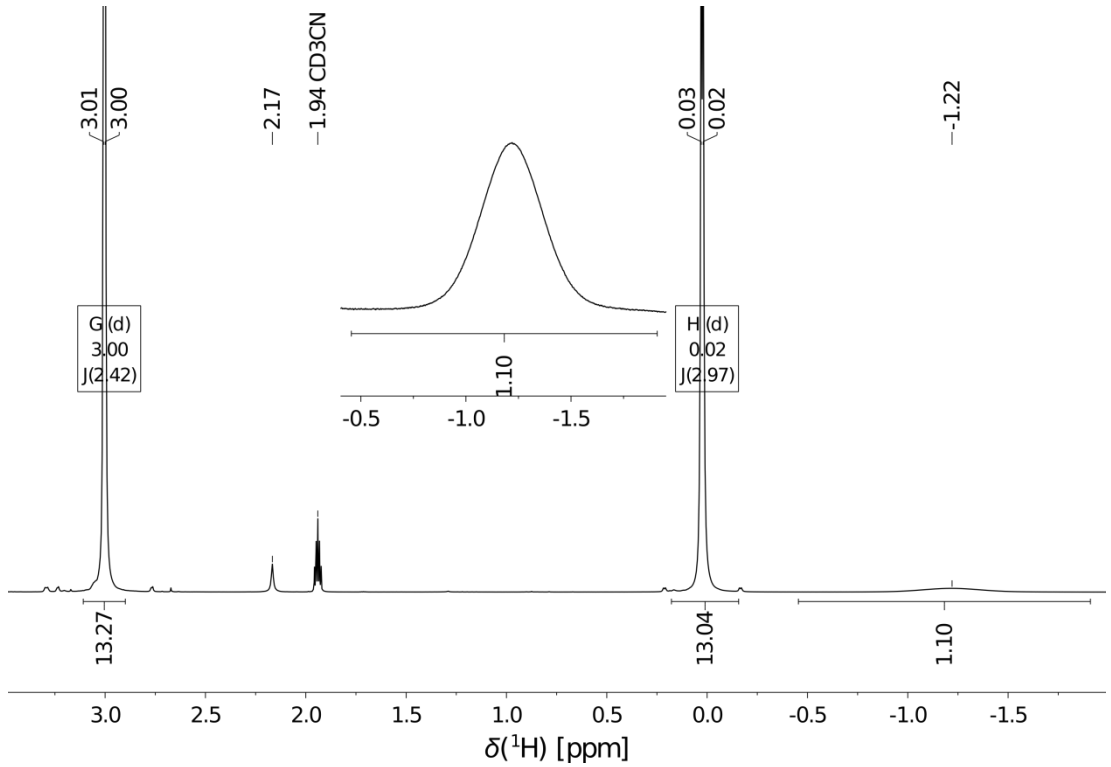


Figure S62. Excerpt of the ^{1}H NMR spectrum (300 MHz, CD_3CN) of [**1**-H][**3**-H] containing the signals of the protons of the methyl groups as well as B*H*B.

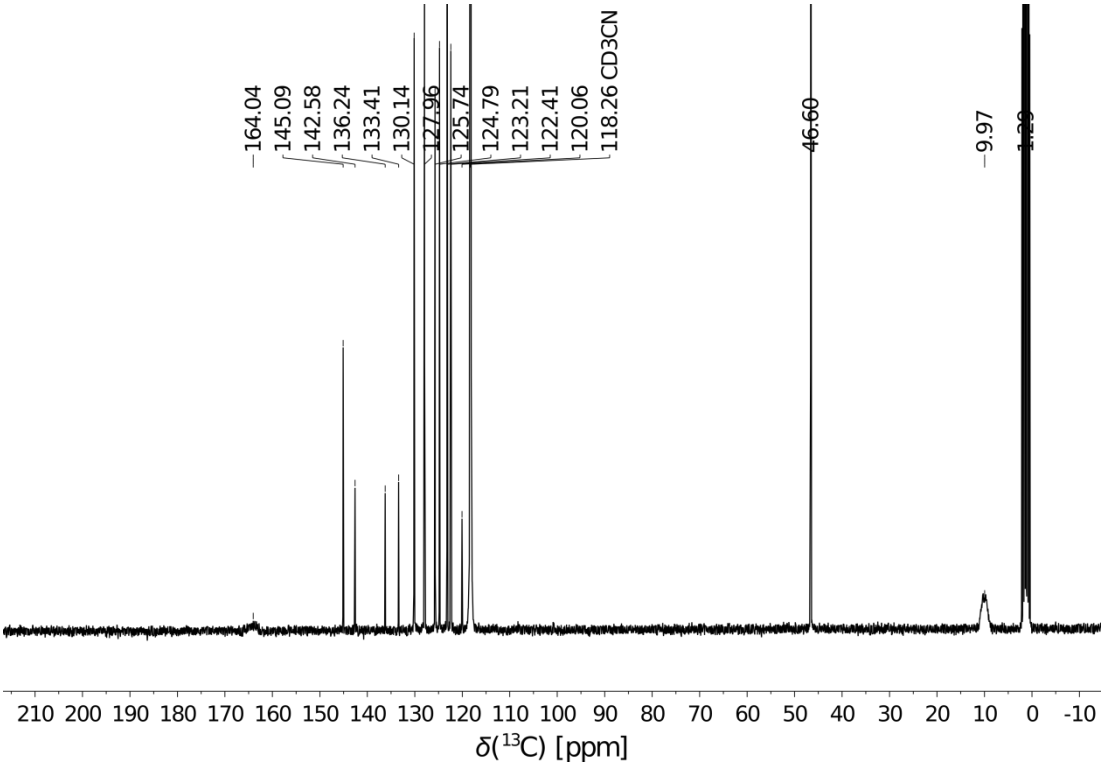


Figure S63. Full $^{13}C\{^{1}H\}$ NMR spectrum (75 MHz, CD_3CN) of [**1**-H][**3**-H].

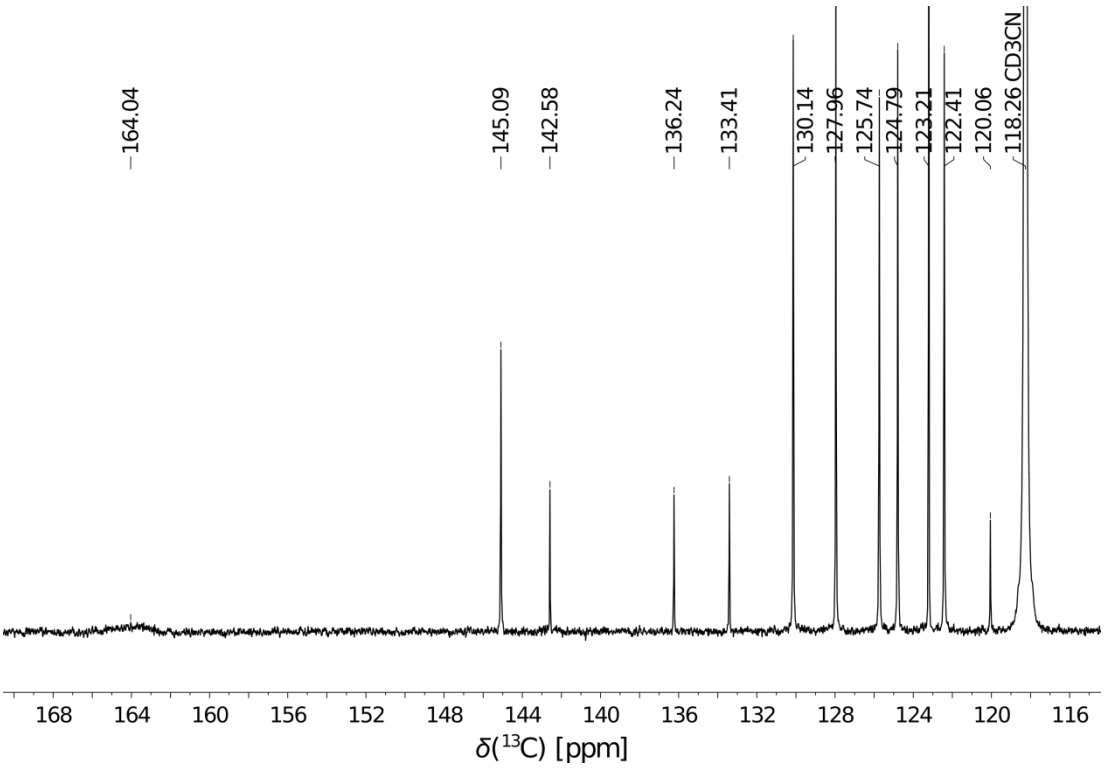


Figure S64. Excerpt of the $^{13}C\{^{1}H\}$ NMR spectrum (75 MHz, CD_3CN) of [**1**-H][**3**-H].

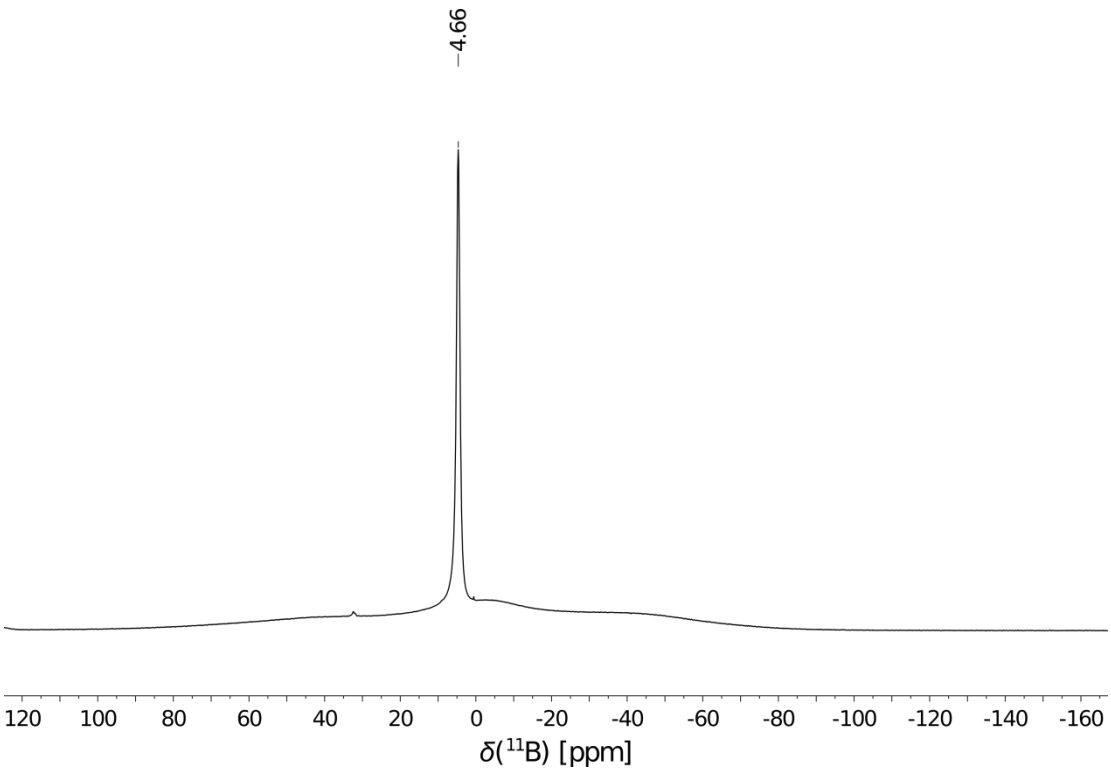


Figure S65. ^{11}B NMR spectrum (96 MHz, CD_3CN) of [**1**-H][**3**-H].

X-Ray crystallography

Single crystals were examined on a Rigaku Supernova diffractometer Using Olex2 [1], the structure was solved with the ShelXT [2] structure solution program using Intrinsic Phasing and refined with the ShelXL [3] refinement package using Least Squares minimization. Details of the X-ray investigation are given in Tables S1-S4. CCDC 2151560–2151570 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via:

www.ccdc.cam.ac.uk/conts/retrieving.html.

1. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, *J. Appl. Crystallogr.* **2009**, 42, 339–341.
2. G. M. Sheldrick, *Acta Crystallogr.* **2015**, *A71*, 3–8.
3. G. M. Sheldrick, *Acta Crystallogr.* **2015**, *C71*, 3–8.

Table S1. Summary of crystallographic data for **1**, the ammonia adduct [**1**-NH_2][**3**-H] and the water adduct [**1**-OH][**3**-H].

compound	**1**	[**1**-NH_2][**3**-H]	[**1**-OH][**3**-H]·MeCN
chemical formula	$C_{14}H_{18}B_2$	$C_{28}H_{39}B_2N_3$	$C_{30}H_{41}B_2N_3O$
M_r	207.90	439.24	481.28
crystal system	orthorhombic	monoclinic	orthorhombic
space group	$P2_12_12_1$	$P2_1/n$	*Pnma*
radiation source	CuKα	CuKα	MoKα
λ (Å)	1.54184	1.54184	0.71073
a (Å)	9.68940(11)	12.0261(3)	17.4262(3)
b (Å)	10.29021(14)	41.6493(15)	9.40374(16)
c (Å)	12.63823(14)	16.3643(4)	17.0884(3)
α (°)	90	90	90
β (°)	90	108.630(3)	90
γ (°)	90	90	90
V (Å^3)	1260.11(3)	7767.1(4)	2800.30(8)
Z / *Z´*	4/1	12/3	4/0.5
T (K)	100.0(1)	100.0(1)	100.0(2)
ρ_{calc} (g cm^{-3})	1.096	1.127	1.142
μ (mm^{-1})	0.430	0.486	0.068
2Θ-range [°]	11.088–152.274	6.082–157.08	3.338–64.508
Index range *h*	−12 to 12	−15 to 15	−25 to 25
Index range *k*	−12 to 12	−52 to 43	−13 to 14
Index range *l*	−15 to 15	−20 to 20	−25 to 25
Refl. collect.	17567	156033	57640
Indep. refl.	5111	16176	5004
R_{int}	0.0169	0.0718	0.0256
Data/restraints/parameters	5111/0/219	16176/0/947	5004/0/281
R_1, $I>2\sigma(I)$ / all data	0.0346/0.0349	0.0800/0.916	0.0417/0.0465
wR_2, $I>2\sigma(I)$ / all data	0.0941/0.0943	0.2069/0.2158	0.1120/0.1154
GoF	1.050	1.073	1.069
$\rho_{max/min}$ [*e* Å^{-3}]	0.26/−0.19	0.33/−0.32	0.45/−0.17
Flack parameter	0.0(3)	-	-
Remarks	Crystal was a three component twin, ratio refined to 61:23:16. All three domains were taken into account during data reduction and refinement. Hydrogen atoms were refined isotropically.	Hydrogen atoms bonded to carbon were taken into account using a riding model, all other ones were refined isotropically.	All hydrogen atoms were refined isotropically.
CCDC	2151560	2151561	2151562

[a] R_1 is defined as $\Sigma||F_o|-|F_c||/\Sigma|F_o|$ for $I>2\sigma(I)$. [b] wR_2 is defined as $[\Sigma w\{F_o^2-F_c^2\}^2/\Sigma w(F_o^2)^2]^{1/2}$ for $I>2\sigma(I)$.

Table S2. Summary of crystallographic data for [**1**-PH_2][**3**-H], [**1**-SH][**3**-H] and [**1**-she][**3**-H].

compound	[**1**-PH_2][**3**-H]	[**1**-SH][**3**-H]	[**1**-SeH][**3**-H]
chemical formula	$C_{28}H_{39}B_2N_2P$	$C_{28}H_{38}B_2N_2S$	$C_{28}H_{38}B_2N_2Se$
M_r	456.20	456.28	503.18
crystal system	triclinic	monoclinic	monoclinic
space group	$P\bar{1}$	$P2_1/n$	$P2_1/n$
radiation source	CuKα	CuKα	MoKα
λ (Å)	1.54184	1.54184	0.71073
a (Å)	12.1822(5)	9.8318(1)	9.84533(19)
b (Å)	13.9482(7)	24.3010(2)	24.1693(4)
c (Å)	16.4722(6)	11.7375(1)	11.8937(2)
α (°)	90.861(3)	90	90
β (°)	107.767(4)	108.063(1)	107.928(2)
γ (°)	91.957(4)	90	90
V (Å^3)	2662.9(2)	2666.14(4)	2692.74(10)
Z / Z'	4/2	4/1	4/1
T (K)	99.97(15)	100.0(1)	100.0(1)
ρ_{calc} (g cm^{-3})	1.138	1.137	1.241
μ (mm^{-1})	1.029	1.191	1.412
2Θ-range [°]	5.636−145.552	7.276−144.692	3.37−64.628
Index range h	−15 to 15	−12 to 12	−14 to 14
Index range k	−17 to 17	−30 to 30	−36 to 36
Index range l	−20 to 20	−14 to 14	−17 to 17
Refl. collect.	36514	37991	131345
Indep. refl.	14775	5265	9163
R_{int}	0.0323	0.0260	0.0477
Data/restraints/param.	14775/0/636	5265/29/334	9163/29/336
R_1, I>2σ(I) / all data	0.0404/0.0515	0.0354/0.0366	0.0383/0.0525
wR_2, I>2σ(I) / all data	0.1038/0.1076	0.0947/0.0956	0.0943/0.0996
GoF	0.948	1.043	1.079
$\rho_{max/min}$ [e Å^{-3}]	0.50/−0.30	0.26/−0.34	0.85/−0.48
Remarks	Refined as a two-component twin. Component 2 rotated by -180.0° around [-0.00 1.00 0.00] (reciprocal) or [0.05 1.00 0.02] (direct). Hydrogens bonded to nitrogen and phosphor were refined isotropically.	Disordered SH-bridge and corresponding methyl groups over two sites, ratio 94:6. H1 and H1a were refined isotropically. H1B was fixed on a reasonable position, all atoms part 2 were refined to have same bond length and displacement parameters as part 1.	Disorder of SeH-bridge and corresponding methyl groups over two sites (94:6). H1 and H1A were refined isotropically. H1B was fixed on a reasonable position, all atoms of part 2 were refined to have same bond length and displacement parameters as part 1.
CCDC	2151563	2151564	2151565

[a] R_1 is defined as $\Sigma||F_o|-|F_c||/\Sigma|F_o|$ for I >2σ(I). [b] wR_2 is defined as$[\Sigma w\{F_o^2-F_c^2\}^2/\Sigma w(F_o^2)^2]^{1/2}$ for I >2σ(I).

Table S3. Summary of crystallographic data for [**1**-CN][**3**-H], [**2**-PH_2][**3**-H] and [**2**-N=C(AsH_2)CH_3][**3**-H]

compound	2([**1**-CN][**3**-H])·MeCN	[**2**-PH_2][**3**-H]	[**2**-N=C(CD_3)AsH_2][**3**-H]
chemical formula	$C_{60}H_{77}B_4N_7$	$C_{24}H_{37}B_2N_2P$	$C_{26}H_{40}B_2N_3As$
M_r	939.52	406.14	491.15
crystal system	triclinic	triclinic	triclinic
space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
radiation source	CuKα	CuKα	CuKα
λ (Å)	1.54184	1.54184	1.54184
a (Å)	9.8110(5)	9.2999(6)	10.1038(4)
b (Å)	16.5987(7)	11.8087(6)	11.6718(4)
c (Å)	17.3054(7)	12.2905(8)	12.9599(4)
α (°)	81.602(4)	63.869(6)	64.302(3)
β (°)	85.872(4)	83.717(6)	88.211(3)
γ (°)	85.229(4)	81.570(5)	78.193(3)
V (Å^3)	2773.2(2)	1197.15(14)	1345.17(9)
Z / Z'	2/1	2/1	2/1
T (K)	100.0(1)	100.0(1)	100.0(1)
ρ_{calc}(g cm^{-3})	1.125	1.127	1.213
μ (mm^{-1})	0.492	1.084	1.822
2Θrange [°]	5.172–152.91	8.022–152.878	7.586–144.252
Index range h	−12 to 9	−10 to 11	−11 to 12
Index range k	−20 to 20	−14 to 13	−14 to 14
Index range l	−21 to 20	−14 to 15	−15 to 15
Refl. collect.	24263	9697	20081
Indep. refl.	11398	4917	5261
R_{int}	0.0379	0.0270	0.0303
Data/restraints/ parameters	11398/0/658	4917/0/414	5261/1/317
R_1, I>2σ(I) / all data	0.0482/0.0633	0.0349/0.0427	0.0454/0.0526
wR_2, I>2σ(I) / all data	0.1223/0.1366	0.0855/0.0906	0.1203/0.1265
GoF	1.013	1.024	1.030
$\rho_{max/min}$ [e Å^{-3}]	0.31/−0.23	0.35/−0.33	0.58/−0.69
Remarks	All hydrogen atoms were taken into account using a riding model. Hydrogen atoms bonded to C60 (methyl groups of solvent can) were refined as idealized disordered methyl group.	All hydrogen atoms were refined isotropically including the disordered one bonded at nitrogen, ratio refines to 65:35.	Disorder of the $AsMe_2$ unit over two sites (81:19). Suitable restraints and constraints were applied, e.g. all As-H distances were restrained to be same.
CCDC	2151566	2151567	2151568

[a] R_1 is defined as $\Sigma||F_o|-|F_c||/\Sigma|F_o|$ for I >2σ(I). [b] wR_2 is defined as $[\Sigma w\{F_o^2-F_c^2\}^2/\Sigma w(F_o^2)^2]^{1/2}$ for I >2 σ(I).

Table S4. Summary of crystallographic data for the formal hydrogen adduct [**1**-H][**3**-H] and the reaction product of **1** with Verkade's base **4**

compound	[**1**-H][**3**-H]	[**4**][**V**-**H**]
chemical formula	$C_{28}H_{38}B_2N_2$	$C_{32}H_{54}B_2N_4P$
M_r	424.22	547.38
crystal system	triclinic	triclinic
space group	$P\bar{1}$	$P\bar{1}$
radiation source	MoKα	CuKα
λ (Å)	0.71073	1.54184
a (Å)	12.06495(18)	9.8912(2)
b (Å)	14.3416(2)	10.6797(3)
c (Å)	15.7603(2)	15.5211(5)
α (°)	90.0174(12)	93.079(2)
β (°)	90.4587(13)	92.337(2)
γ (°)	110.2753(14)	94.679(2)
V (Å^3)	2557.95(7)	1630.07(8)
Z / Z'	4 / 2	2 / 1
T (K)	200.0(1)	100.0(1)
ρ_{calc} (g cm^{-3})	1.102	1.115
μ (mm^{-1})	0.062	0.928
2Θ-range [°]	3.028–72.636	5.708–153.114
Index range h	−20 to 19	−12 to 7
Index range k	−23 to 23	−12 to 13
Index range l	−26 to 26	−19 to 18
Refl. collect.	249239	13361
Indep. refl.	24769	6713
R_{int}	0.0395	0.0395
Data/restraints/parameters	24769/0/882	6713/18/384
R_1, I>2σ(I) / all data	0.0573/0.0869	0.0499/0.0525
wR_2, I>2σ(I) / all data	0.1588/0.1754	0.1377/0.1412
GoF	1.018	1.034
$\rho_{max/min}$ [e Å^{-3}]	0.42/−0.23	0.51/−0.47
Remarks	All hydrogen atoms were refined isotropically.	The hydrogen atom H1 bonded to P1 was refined isotropically, for all other ones a riding model was applied. One i-propylgroup is disordered over two sites with ratio 1:1.
CCDC	2151569	2151570

[a] R_1 is defined as $\Sigma||F_o|-|F_c||/\Sigma\ |F_o|$ for I >2σ(I). [b] wR_2 is defined as$[\Sigma w\{F_o^2-F_c^2\}^2/\Sigma w(F_o^2)^2]^{1/2}$ for I >2 σ(I).

Gas-phase electron diffraction

Table S5. Cartesian coordinates of the gas-phase structure of **1**

Number	Atom	Atomic Number	Mass	*X*	*Y*	*Z*
1	X	−1	0.00000000	0.649998140879	0.060348749199	−0.998887471114
2	C	6	12.00000000	0.649499141527	0.000462599016	−0.000682381959
3	C	6	12.00000000	2.083522276427	0.002283173778	0.000143704622
4	C	6	12.00000000	−0.038684050056	−1.256332740298	−0.076426373075
5	C	6	12.00000000	−0.041959782844	1.255506403395	0.074266849429
6	C	6	12.00000000	0.722087333773	−2.420424366274	−0.145884385527
7	C	6	12.00000000	0.715772862903	2.421525857484	0.144599614715
8	C	6	12.00000000	2.127574422197	−2.407912654897	−0.144431161747
9	C	6	12.00000000	2.121287930764	2.412582874851	0.144765703136
10	C	6	12.00000000	2.800924841859	−1.215434196544	−0.072553201748
11	C	6	12.00000000	2.797746379098	1.221818076411	0.073665317058
12	B	5	11.00930550	−1.579829212269	−1.477278816993	−0.050786928587
13	B	5	11.00930550	−1.583630420868	1.472538668307	0.046851511163
14	C	6	12.00000000	−2.557980951011	−0.483549468081	−0.772616366868
15	H	1	1.00782503	−2.737189328941	−0.935443447506	−1.755014171700
16	H	1	1.00782503	−2.116238379746	0.488968171603	−0.985652645992
17	H	1	1.00782503	−3.535021361548	−0.347141477618	−0.319767734011
18	C	6	12.00000000	−2.210674235193	−2.837493182667	0.408582285917
19	H	1	1.00782503	−2.802291217641	−2.642017011678	1.306385097012
20	H	1	1.00782503	−2.924739872449	−3.228124034758	−0.316888185250
21	H	1	1.00782503	−1.502058152963	−3.620803435759	0.664285298237
22	C	6	12.00000000	−2.560044017966	0.476297768308	0.767571385619
23	H	1	1.00782503	−2.741525295033	0.927725995226	1.749764934835
24	H	1	1.00782503	−2.116071851463	−0.495099376922	0.981089522917
25	H	1	1.00782503	−3.536222598717	0.337417781293	0.313619246429
26	C	6	12.00000000	−2.217053562343	2.834978047130	−0.402261728061
27	H	1	1.00782503	−2.806039189434	2.645796092447	−1.303130464428
28	H	1	1.00782503	−2.933898536312	3.217305393180	0.324899842489
29	H	1	1.00782503	−1.511575184761	3.636900186169	−0.603041531980
30	H	1	1.00782503	0.216651201031	−3.373793979164	−0.203333349416
31	H	1	1.00782503	0.207851796388	3.373608955186	0.201464821784
32	H	1	1.00782503	2.674786014693	−3.336700090507	−0.199879131536
33	H	1	1.00782503	2.666075219834	3.342756665783	0.200842732248
34	H	1	1.00782503	3.881346833165	−1.190341092865	−0.070507670954
35	H	1	1.00782503	3.878230241395	1.199468366869	0.072864602531

Table S6. Full listing of structural parameters of the refined gas-phase structure of **1**. r_a, r_g, r_e values are given in Å. For atom numbering, see Table S5.

Number	Type	Atom 1	Atom2	Atom 3	Atom4	r_a	r_g	r_e	3σ
1	stretch	1	2	0	0	1.00000	1.00000	1.00000	0.00000
2	stretch	2	3	0	0	1.43052	1.43236	1.43402	0.00018
3	stretch	2	4	0	0	1.43348	1.43532	1.43488	0.00018
4	stretch	2	5	0	0	1.43348	1.43532	1.43488	0.00018
5	stretch	3	10	0	0	1.41490	1.41665	1.41520	0.00018
6	stretch	3	11	0	0	1.41490	1.41665	1.41520	0.00018
7	stretch	4	6	0	0	1.39207	1.39378	1.39237	0.00018
8	stretch	4	12	0	0	1.55681	1.55870	1.55711	0.00059
9	stretch	5	7	0	0	1.39207	1.39378	1.39237	0.00018
10	stretch	5	13	0	0	1.55681	1.55870	1.55711	0.00059
11	stretch	6	8	0	0	1.40624	1.40799	1.40554	0.00018
12	stretch	6	30	0	0	1.07899	1.08479	1.08059	0.00075
13	stretch	7	9	0	0	1.40634	1.40809	1.40554	0.00018
14	stretch	7	31	0	0	1.07899	1.08479	1.08059	0.00075
15	stretch	8	10	0	0	1.37184	1.37346	1.37134	0.00018
16	stretch	8	32	0	0	1.07773	1.08350	1.07943	0.00075
17	stretch	9	11	0	0	1.37184	1.37346	1.37134	0.00018
18	stretch	9	33	0	0	1.07773	1.08350	1.07943	0.00075
19	stretch	10	34	0	0	1.07892	1.08472	1.08072	0.00075
20	stretch	11	35	0	0	1.07892	1.08472	1.08072	0.00075
21	stretch	12	14	0	0	1.56983	1.57179	1.57013	0.00059
22	stretch	12	18	0	0	1.56717	1.56912	1.56817	0.00059
23	stretch	13	22	0	0	1.56983	1.57179	1.57013	0.00059
24	stretch	13	26	0	0	1.56717	1.56912	1.56817	0.00059
25	stretch	14	15	0	0	1.09450	1.10052	1.09610	0.00075
26	stretch	14	16	0	0	1.08748	1.09340	1.08918	0.00075
27	stretch	14	17	0	0	1.08389	1.08977	1.08549	0.00075
28	stretch	18	19	0	0	1.09113	1.09715	1.09283	0.00075
29	stretch	18	20	0	0	1.08842	1.09439	1.09032	0.00075
30	stretch	18	21	0	0	1.08518	1.09109	1.08678	0.00075
31	stretch	22	23	0	0	1.09450	1.10052	1.09610	0.00075
32	stretch	22	24	0	0	1.08748	1.09342	1.08918	0.00075
33	stretch	22	25	0	0	1.08389	1.08977	1.08549	0.00075
34	stretch	26	27	0	0	1.09112	1.09713	1.09282	0.00075
35	stretch	26	28	0	0	1.08842	1.09440	1.09032	0.00075
36	stretch	26	29	0	0	1.08528	1.09118	1.08678	0.00075
37	bend	1	2	3	0			90.00000	0.00000
38	bend	1	2	4	0			90.00000	0.00000
39	bend	1	2	5	0			90.00000	0.00000
40	bend	3	2	4	0			118.73464	0.02511
41	bend	3	2	5	0			118.73464	0.02511
42	bend	2	3	10	0			120.38478	0.12619
43	bend	2	3	11	0			120.38478	0.12619
44	bend	4	2	5	0			122.53072	0.05022
45	bend	2	4	6	0			118.22064	0.02511
46	bend	2	4	12	0			126.73454	0.13103
47	bend	2	5	7	0			118.22064	0.02511
48	bend	2	5	13	0			126.73454	0.13103
49	bend	10	3	11	0			119.23043	0.25239
50	bend	3	10	8	0			120.13321	0.18020
51	bend	3	10	34	0			119.12479	0.18020
52	bend	3	11	9	0			120.13321	0.18020
53	bend	3	11	35	0			119.12479	0.18020
54	bend	6	4	12	0			115.02234	0.13546
55	bend	4	6	8	0			122.60664	0.02511
56	bend	4	6	30	0			118.99300	0.00000
57	bend	4	12	14	0			121.27934	0.17551
58	bend	4	12	18	0			121.73934	0.17551
59	bend	7	5	13	0			115.02234	0.13546
60	bend	5	7	9	0			122.60664	0.02511
61	bend	5	7	31	0			118.99300	0.00000

62	bend	5	13	22	0			121.27734	0.17551
63	bend	5	13	26	0			121.73934	0.17551
64	bend	8	6	30	0			118.40036	0.02511
65	bend	6	8	10	0			119.92009	0.12933
66	bend	6	8	32	0			119.94800	0.00000
67	bend	9	7	31	0			118.40036	0.02511
68	bend	7	9	11	0			119.92009	0.12933
69	bend	7	9	33	0			119.94800	0.00000
70	bend	10	8	32	0			120.13191	0.12933
71	bend	8	10	34	0			120.74200	0.00000
72	bend	11	9	33	0			120.13191	0.12933
73	bend	9	11	35	0			120.74200	0.00000
74	bend	14	12	18	0			115.65962	0.31213
75	bend	12	14	15	0			104.65300	0.00000
76	bend	12	14	16	0			113.72600	0.00000
77	bend	12	14	17	0			116.64600	0.00000
78	bend	12	18	19	0			107.65500	0.00000
79	bend	12	18	20	0			112.29100	0.00000
80	bend	12	18	21	0			115.58200	0.00000
81	bend	22	13	26	0			115.56441	0.31375
82	bend	13	22	23	0			104.65300	0.00000
83	bend	13	22	24	0			113.72700	0.00000
84	bend	13	22	25	0			116.64500	0.00000
85	bend	13	26	27	0			107.66100	0.00000
86	bend	13	26	28	0			112.28500	0.00000
87	bend	13	26	29	0			115.58100	0.00000
88	bend	15	14	16	0			105.01800	0.00000
89	bend	15	14	17	0			106.17400	0.00000
90	bend	16	14	17	0			109.53892	0.00000
91	bend	19	18	20	0			104.84300	0.00000
92	bend	19	18	21	0			106.77500	0.00000
93	bend	20	18	21	0			108.98674	0.00000
94	bend	23	22	24	0			105.01900	0.00000
95	bend	23	22	25	0			106.17300	0.00000
96	bend	24	22	25	0			109.53898	0.00000
97	bend	27	26	28	0			104.84100	0.00000
98	bend	27	26	29	0			108.98400	0.00000
99	bend	28	26	29	0			106.93316	0.00000
100	torsion	1	2	3	10			−90.00000	0.00000
101	torsion	1	2	3	11			90.00000	0.00000
102	torsion	1	2	4	6			90.00000	0.00000
103	torsion	1	2	4	12			−91.81823	0.94355
104	torsion	1	2	5	7			−90.00000	0.00000
105	torsion	1	2	5	13			88.18177	0.94355
106	torsion	10	3	2	4			0.00000	0.00000
107	torsion	11	3	2	4			−180.00000	0.00000
108	torsion	3	2	4	6			0.00000	0.00000
109	torsion	3	2	4	12			178.18177	0.94355
110	torsion	10	3	2	5			−180.00000	0.00000
111	torsion	11	3	2	5			0.00000	0.00000
112	torsion	3	2	5	7			0.00000	0.00000
113	torsion	3	2	5	13			178.18177	0.94355
114	torsion	2	3	10	8			−0.00000	0.00000
115	torsion	2	3	10	34			−180.00000	0.00000
116	torsion	2	3	11	9			−0.00000	0.00000
117	torsion	2	3	11	35			−180.00000	0.00000
118	torsion	6	4	2	5			180.00000	0.00000
119	torsion	12	4	2	5			−1.81823	0.94355
120	torsion	4	2	5	7			−180.00000	0.00000
121	torsion	4	2	5	13			−1.81823	0.94355
122	torsion	2	4	6	8			−0.00000	0.00000
123	torsion	2	4	6	30			180.00000	0.00000
124	torsion	2	4	12	14			37.71252	1.10930
125	torsion	2	4	12	18			−155.98651	1.47825
126	torsion	2	5	7	9			−0.00000	0.00000

127	torsion	2	5	7	31			180.00000	0.00000
128	torsion	2	5	13	22			37.71252	1.10930
129	torsion	2	5	13	26			−156.48651	1.47825
130	torsion	8	10	3	11			180.00000	0.00000
131	torsion	10	3	11	9			180.00000	0.00000
132	torsion	34	10	3	11			0.00000	0.00000
133	torsion	10	3	11	35			0.00000	0.00000
134	torsion	3	10	8	6			0.00000	0.00000
135	torsion	3	10	8	32			−180.00000	0.00000
136	torsion	3	11	9	7			0.00000	0.00000
137	torsion	3	11	9	33			−180.00000	0.00000
138	torsion	8	6	4	12			−178.39198	0.83502
139	torsion	30	6	4	12			1.60802	0.83502
140	torsion	6	4	12	14			−144.05551	0.80438
141	torsion	6	4	12	18			22.24547	1.32264
142	torsion	4	6	8	10			−0.00000	0.00000
143	torsion	4	6	8	32			180.00000	0.00000
144	torsion	4	12	14	15			95.14993	0.70486
145	torsion	4	12	14	16			−18.89664	0.70486
146	torsion	4	12	14	17			−147.89264	0.70486
147	torsion	4	12	18	19			116.72282	0.70771
148	torsion	4	12	18	20			−128.37805	0.70771
149	torsion	4	12	18	21			−2.49740	0.70771
150	torsion	9	7	5	13			−178.39198	0.83502
151	torsion	31	7	5	13			1.60802	0.83502
152	torsion	7	5	13	22			−144.05551	0.80438
153	torsion	7	5	13	26			21.74547	1.32264
154	torsion	5	7	9	11			−0.00000	0.00000
155	torsion	5	7	9	33			180.00000	0.00000
156	torsion	5	13	22	23			95.14993	0.70486
157	torsion	5	13	22	24			−18.89831	0.70486
158	torsion	5	13	22	25			−147.89444	0.70486
159	torsion	5	13	26	27			116.72282	0.70771
160	torsion	5	13	26	28			−128.38012	0.70771
161	torsion	5	13	26	29			−5.34441	0.70771
162	torsion	10	8	6	30			−180.00000	0.00000
163	torsion	32	8	6	30			0.00000	0.00000
164	torsion	6	8	10	34			180.00000	0.00000
165	torsion	11	9	7	31			−180.00000	0.00000
166	torsion	33	9	7	31			−0.00000	0.00000
167	torsion	7	9	11	35			180.00000	0.00000
168	torsion	34	10	8	32			−0.00000	0.00000
169	torsion	35	11	9	33			−0.00000	0.00000
170	torsion	15	14	12	18			−71.93890	1.32955
171	torsion	16	14	12	18			174.01453	1.32955
172	torsion	17	14	12	18			45.01852	1.32955
173	torsion	14	12	18	19			−76.25315	1.36096
174	torsion	14	12	18	20			38.64597	1.36096
175	torsion	14	12	18	21			164.52662	1.36096
176	torsion	23	22	13	26			−71.47960	1.32788
177	torsion	24	22	13	26			174.47216	1.32788
178	torsion	25	22	13	26			45.47603	1.32788
179	torsion	22	13	26	27			−76.71514	1.35930
180	torsion	22	13	26	28			38.18192	1.35930
181	torsion	22	13	26	29			161.21763	1.35930
182	o.o.p	34	3	10	8			0.00000	0.00000
183	o.o.p	35	3	11	9			0.00000	0.00000
184	o.o.p	30	4	6	8			−0.00000	0.00000
185	o.o.p	31	5	7	9			−0.00000	0.00000
186	o.o.p	32	6	8	10			0.00000	0.00000
187	o.o.p	33	7	9	11			−0.00000	0.00000

Table S7. Listing of interatomic distances for **1** of r_a type along with the amplitude *l* and the amplitude correction corr, due to thermal motion. The group the amplitudes were refined in are given in the last column.

Atom 1	Atom 2	r_a	*l*	Corr	Group
C9	H33	1.077726	0.078909	0.001700	100
C8	H32	1.077726	0.078909	0.001700	100
C10	H34	1.078915	0.079116	0.001800	100
C11	H35	1.078915	0.079116	0.001800	100
C6	H30	1.078992	0.079116	0.001600	100
C7	H31	1.078992	0.079116	0.001600	100
C22	H25	1.083888	0.079838	0.001600	100
C14	H17	1.083889	0.079838	0.001600	100
C18	H21	1.085182	0.080045	0.001600	100
C26	H29	1.085280	0.080045	0.001500	100
C14	H16	1.087479	0.080251	0.001700	100
C22	H24	1.087480	0.080354	0.001700	100
C18	H20	1.088416	0.080664	0.001900	100
C26	H28	1.088423	0.080664	0.001900	100
C26	H27	1.091121	0.080976	0.001700	100
C18	H19	1.091127	0.081077	0.001700	100
C22	H23	1.094496	0.081181	0.001600	100
C14	H15	1.094497	0.081181	0.001600	100
C9	C11	1.371840	0.047150	−0.000500	101
C8	C10	1.371840	0.047150	−0.000500	101
C5	C7	1.392075	0.048740	0.000300	101
C4	C6	1.392075	0.048740	0.000300	101
C6	C8	1.406244	0.049587	−0.000700	101
C7	C9	1.406344	0.049587	−0.000800	101
C3	C10	1.414899	0.049798	0.000300	101
C3	C11	1.414899	0.049798	0.000300	101
C2	C3	1.430525	0.051174	0.003500	101
C2	C4	1.433476	0.051389	0.001400	101
C2	C5	1.433476	0.051389	0.001400	101
B13	H16	1.487818	0.548582	0.034400	103
B12	H24	1.487870	0.548582	0.034300	103
C4	B12	1.556814	0.054232	0.000300	102
C5	B13	1.556814	0.054232	0.000300	102
B12	C18	1.567174	0.055235	0.001000	102
B13	C26	1.567174	0.055235	0.001000	102
B13	C22	1.569833	0.055437	0.000300	102
B12	C14	1.569833	0.055437	0.000300	102
C14	H25	1.631959	0.380100	0.044600	105
H17	C22	1.631986	0.380198	0.044600	105
H27	H28	1.717160	0.173566	0.013000	103
H19	H20	1.717182	0.173700	0.013000	103
H15	H16	1.721111	0.173966	0.012800	103
H23	H24	1.721122	0.174099	0.012800	103
H23	H25	1.731083	0.173299	0.013200	103
H15	H17	1.731096	0.173167	0.013200	103
H19	H21	1.736049	0.173700	0.013500	103
H28	H29	1.736825	0.169298	0.012500	103
H20	H21	1.759765	0.169298	0.012500	103
H27	H29	1.760774	0.173700	0.013500	103
H16	H17	1.764552	0.168230	0.011800	103
H24	H25	1.764553	0.168363	0.011800	103
C14	H24	1.772263	0.460966	0.036300	105
H16	C22	1.772268	0.460966	0.036300	105
C14	C22	1.787097	0.297969	0.027700	105
H16	H25	1.863855	0.506509	0.066800	105
H17	H24	1.863984	0.506606	0.066700	105
H29	H31	1.978603	0.449726	−0.062100	103
H21	H30	2.003566	0.447885	−0.062500	104
B13	H23	2.114330	0.181972	0.015800	103
B12	H15	2.114331	0.181972	0.015800	103

C11	H33	2.121724	0.131677	0.007100	103
C10	H32	2.121724	0.131677	0.007100	103
C8	H34	2.129573	0.131809	0.006700	103
C9	H35	2.129673	0.131809	0.006600	103
C5	H31	2.129773	0.132477	0.006800	103
C4	H30	2.129773	0.132477	0.006800	103
C9	H31	2.134967	0.133142	0.007000	103
C8	H30	2.135067	0.133142	0.006900	103
C7	H33	2.150463	0.133678	0.007200	103
C6	H32	2.150463	0.133678	0.007200	103
B12	H19	2.151420	0.182504	0.014900	103
C3	H34	2.151492	0.134211	0.007100	103
C3	H35	2.151492	0.134211	0.007100	103
B13	H27	2.151495	0.182372	0.014900	103
H16	H24	2.183196	0.768130	0.016000	106
B13	H28	2.214078	0.168764	0.009600	103
B12	H20	2.214148	0.168764	0.009600	103
B12	H16	2.235584	0.159559	0.006700	103
B13	H24	2.235597	0.159559	0.006700	103
B13	H29	2.253076	0.154222	0.007900	103
B12	H21	2.253090	0.154355	0.007900	103
B13	H25	2.267165	0.152754	0.007100	103
B12	H17	2.267177	0.152754	0.007100	103
B13	C14	2.327617	0.217200	0.006300	105
B12	C22	2.327679	0.217200	0.006200	105
H19	H24	2.368772	0.567181	−0.091500	103
H16	H27	2.377597	0.575000	−0.091000	103
C18	H24	2.386598	0.464447	0.026600	104
H34	H35	2.392208	0.259349	0.001900	103
H16	C26	2.392860	0.464447	0.026700	104
C7	C11	2.402243	0.057238	0.001700	104
C6	C10	2.402243	0.057238	0.001700	104
C5	H16	2.404073	0.332552	0.048200	104
C4	H24	2.404215	0.332351	0.048000	104
C3	C9	2.410530	0.056729	0.004400	104
C3	C8	2.410730	0.056729	0.004200	104
C2	C6	2.421324	0.058052	0.005000	104
C2	C7	2.421324	0.058052	0.005000	104
C10	C11	2.437036	0.063135	0.004600	104
H31	H33	2.446217	0.165209	0.012200	104
H30	H32	2.446317	0.165209	0.012100	104
C4	C8	2.451569	0.057748	0.002700	104
C5	C9	2.451669	0.057748	0.002600	104
H32	H34	2.454140	0.164498	0.011500	104
H33	H35	2.454340	0.164498	0.011300	104
C3	C5	2.462950	0.059476	0.005600	104
C3	C4	2.463050	0.059476	0.005500	104
C2	C10	2.467487	0.059170	0.004800	104
C2	C11	2.467787	0.059170	0.004500	104
H15	H25	2.475127	0.440122	0.081800	107
H17	H23	2.475130	0.439899	0.081800	107
C6	B12	2.484155	0.079504	0.005300	104
C7	B13	2.484155	0.079504	0.005300	104
C4	C5	2.510457	0.064762	0.005900	104
C26	H31	2.564121	0.199617	−0.007800	105
C18	H30	2.567872	0.199617	−0.007800	105
B13	H31	2.608950	0.150569	0.007800	104
B12	H30	2.608950	0.150569	0.007800	104
C11	H34	2.639799	0.137455	0.008500	104
C10	H35	2.639899	0.137455	0.008400	104
C22	C26	2.650294	0.085909	0.004800	104
C14	C18	2.651683	0.086009	0.004800	104
C2	B13	2.671095	0.073200	0.004000	104
C2	B12	2.671095	0.073200	0.004000	104
B12	H25	2.682912	0.339716	0.010300	105

B13	H17	2.682946	0.339716	0.010300	105
C7	H29	2.709119	0.242988	−0.063900	105
C5	C22	2.715543	0.080769	0.010000	105
C4	C14	2.715670	0.080769	0.009900	105
C6	H21	2.718274	0.243085	−0.064200	105
C4	C18	2.728690	0.076390	0.001300	105
C5	C26	2.728690	0.076390	0.001300	105
H15	H24	2.759362	0.552571	0.080700	107
H16	H23	2.759371	0.552238	0.080700	107
H23	H28	2.767394	0.350017	−0.063800	105
C3	C7	2.776266	0.062280	0.006600	105
C3	C6	2.776566	0.062280	0.006300	105
H15	H20	2.776989	0.350116	−0.064100	105
H15	C22	2.817975	0.343355	0.078200	107
C14	H23	2.818069	0.342910	0.078100	107
C2	C8	2.822624	0.062280	0.006800	105
C2	C9	2.822724	0.062280	0.006700	105
C22	H28	2.823780	0.207079	−0.022200	105
C5	H24	2.825923	0.134193	0.035700	105
C4	H16	2.825943	0.134485	0.035700	105
C14	H20	2.828623	0.207079	−0.022400	105
C4	C10	2.836006	0.062475	0.003900	105
C5	C11	2.836306	0.062475	0.003600	105
H17	H19	2.872996	0.241625	0.033500	105
H25	H27	2.877798	0.241430	0.033500	105
H17	C18	2.884315	0.111422	0.028800	105
H25	C26	2.885046	0.111324	0.028800	105
H23	C26	2.906495	0.212627	0.016500	105
H15	C18	2.912008	0.212627	0.016500	105
C4	H21	2.913545	0.180611	−0.035900	105
C5	H29	2.914858	0.180513	−0.035700	105
H25	H28	2.918023	0.206107	0.024200	105
H17	H20	2.920813	0.206302	0.024100	105
C2	H16	2.927957	0.216130	0.048300	105
C2	H24	2.928012	0.215838	0.048200	105
B12	B13	2.952235	0.148596	−0.000800	105
C14	H19	2.990912	0.248048	0.015900	105
C22	H27	2.993360	0.247659	0.015800	105
C7	C26	3.012088	0.120959	−0.000200	105
C6	C18	3.013814	0.120959	−0.000100	105
H20	H24	3.025491	0.734380	0.106300	106
H16	H28	3.029274	0.733746	0.106000	106
H20	H30	3.058416	0.490452	0.088400	105
H28	H31	3.060157	0.489674	0.087900	105
H21	H24	3.115857	0.547985	0.085300	105
C5	B12	3.132579	0.102761	0.005700	105
C4	B13	3.132679	0.102761	0.005600	105
H16	H29	3.143032	0.547886	0.085200	105
C5	H23	3.144218	0.245420	0.049900	105
C4	H15	3.144244	0.245518	0.049900	105
B13	H15	3.155048	0.279956	0.066100	107
B12	H23	3.155214	0.279178	0.065900	107
C5	C14	3.163224	0.213158	0.010400	106
C4	C22	3.163278	0.213158	0.010300	106
H19	H25	3.196900	0.560461	0.028200	104
H17	H27	3.205388	0.559861	0.028200	104
H19	C22	3.228382	0.436342	−0.054600	105
C14	H27	3.237974	0.435647	−0.054300	105
C4	H19	3.315611	0.358435	0.071100	106
C5	H27	3.315978	0.357801	0.070800	106
C2	C22	3.321737	0.158727	0.012600	106
C2	C14	3.321778	0.158727	0.012600	106
C18	C22	3.346739	0.324685	0.004700	106
H27	H31	3.348211	0.323223	0.098100	107
C14	C26	3.351789	0.324685	0.004700	106

H19	H30	3.355304	0.323446	0.098500	107
C10	H30	3.357683	0.121805	0.011900	106
C11	H31	3.357683	0.121805	0.011900	106
C6	H34	3.379522	0.121170	0.011600	106
C7	H35	3.379622	0.121170	0.011500	106
C3	H33	3.382824	0.121170	0.014000	106
C3	H32	3.383024	0.121170	0.013800	106
C2	H31	3.393937	0.121931	0.014000	106
C2	H30	3.393937	0.121931	0.014000	106
C4	H32	3.408216	0.122693	0.013200	106
C5	H33	3.408316	0.122693	0.013100	106
H23	H27	3.414326	0.486203	0.089400	106
H15	H19	3.415838	0.486711	0.089700	106
C2	H34	3.429657	0.123708	0.015300	106
C2	H35	3.429857	0.123708	0.015100	106
C18	H25	3.436125	0.381117	0.005700	105
H17	C26	3.439547	0.381117	0.005700	105
C4	H20	3.446984	0.285987	0.056600	106
C5	H28	3.447138	0.285606	0.056400	106
C7	H16	3.553161	0.400414	0.056900	107
C6	H24	3.553299	0.400192	0.056700	107
C22	H29	3.556710	0.138588	0.044300	107
C14	H21	3.564204	0.138699	0.044400	107
H20	H25	3.575130	0.459141	0.097000	107
H17	H28	3.575215	0.459030	0.096600	107
H19	H23	3.604986	0.541338	−0.007300	107
H24	C26	3.609492	0.216891	−0.002100	107
H16	C18	3.610168	0.216891	−0.002100	107
H15	H27	3.617093	0.541004	−0.006800	107
C5	H25	3.618080	0.202320	0.002700	107
C4	H17	3.618204	0.202432	0.002600	107
C6	H20	3.658313	0.440678	0.080800	107
C7	H28	3.659369	0.439899	0.080400	107
C9	C10	3.687918	0.072186	0.009600	107
C8	C11	3.688018	0.072186	0.009500	107
C7	H27	3.714265	0.319998	0.100100	107
C6	H19	3.717803	0.320442	0.100500	107
H23	H29	3.732365	0.295973	0.060800	107
C5	C6	3.750044	0.074077	0.010900	107
C4	C7	3.750044	0.074077	0.010900	107
H15	H21	3.758649	0.296195	0.061000	107
C5	C10	3.759896	0.070740	0.009600	107
C4	C11	3.760196	0.070740	0.009300	107
H20	C22	3.783186	0.377501	0.093900	107
C14	H28	3.784825	0.377057	0.093600	107
C8	B12	3.813470	0.089315	0.010100	107
C9	B13	3.813570	0.089315	0.010000	107
H15	H23	3.829944	0.373509	0.139300	109
H16	H31	3.836061	0.467483	0.053900	107
H24	H30	3.836102	0.467372	0.053800	107
C7	C22	3.840738	0.138699	0.019700	107
C6	C14	3.840757	0.138699	0.019700	107
C3	H31	3.845525	0.106777	0.017700	107
C3	H30	3.845925	0.106777	0.017300	107
H24	H28	3.847538	0.459698	0.010100	107
H16	H20	3.852443	0.459920	0.009900	107
C5	H15	3.853258	0.298642	0.072400	107
C4	H23	3.853413	0.298086	0.072200	107
C2	H15	3.857646	0.327227	0.069600	107
C2	H23	3.857704	0.327005	0.069500	107
C5	H17	3.889018	0.288187	−0.025700	107
C4	H25	3.889083	0.287853	−0.025800	107
C2	H32	3.890324	0.106777	0.018400	107
C2	H33	3.890424	0.106777	0.018300	107
C4	H34	3.904991	0.107000	0.015600	107

C5	H35	3.905191	0.107000	0.015400	107
H17	H21	3.919305	0.169286	0.057900	107
H25	H29	3.920397	0.169286	0.057800	107
C3	B13	3.938982	0.083086	0.012200	107
C3	B12	3.939082	0.083086	0.012100	107
C18	H23	3.964853	0.331454	0.067200	107
H16	H19	3.969153	0.446907	−0.028700	107
C9	H29	3.970875	0.292747	−0.065000	107
H15	C26	3.972076	0.332344	0.067300	107
H24	H27	3.973282	0.446128	−0.028800	107
C8	H21	3.976740	0.292747	−0.065300	107
C9	H34	4.001021	0.151490	0.014600	107
C8	H35	4.001121	0.151490	0.014500	107
C22	H31	4.023444	0.210885	0.023300	107
C14	H30	4.023449	0.210885	0.023300	107
C2	C18	4.037948	0.102217	0.012000	107
C2	C26	4.039280	0.102217	0.012000	107
C7	H23	4.049008	0.348027	0.045000	107
C6	H15	4.049028	0.347915	0.045000	107
C7	H24	4.100493	0.155049	0.049900	107
C6	H16	4.100506	0.155383	0.049900	107
H23	H31	4.103502	0.371718	0.029100	107
H15	H30	4.103507	0.371718	0.029100	107
C7	C10	4.185915	0.076746	0.012000	107
C6	C11	4.186215	0.076746	0.011700	107
H21	C22	4.190558	0.478384	0.042200	107
C14	H29	4.212524	0.478050	0.042100	107
C2	H17	4.225940	0.251037	−0.014900	107
C2	H25	4.226008	0.250815	−0.015000	107
H30	H34	4.245716	0.145817	0.022200	107
H31	H35	4.245816	0.145817	0.022100	107
C5	C8	4.250155	0.077191	0.013100	107
C4	C9	4.250255	0.077191	0.013000	107
C3	H16	4.275672	0.239692	0.065600	107
C3	H24	4.275725	0.239247	0.065500	107
C2	H21	4.283081	0.230905	−0.018700	107
C2	H29	4.291293	0.230794	−0.018500	107
H29	H33	4.329148	0.319111	−0.064700	108
H21	H32	4.339954	0.375546	−0.065200	109
B13	C18	4.359201	0.217113	0.011200	107
B12	C26	4.362031	0.217113	0.011200	107
C10	B12	4.376326	0.088870	0.012300	107
C11	B13	4.376626	0.088870	0.012000	107
C9	C26	4.385347	0.131818	0.007700	108
C8	C18	4.386602	0.131920	0.007800	108
H24	H29	4.404553	0.214166	0.061800	108
H16	H21	4.408888	0.214268	0.062100	108
H21	H25	4.449913	0.589276	0.014200	107
C7	C14	4.454236	0.201646	0.017700	108
C6	C22	4.454289	0.201646	0.017600	108
H17	H29	4.463206	0.588831	0.014200	107
C2	H19	4.473881	0.369716	0.065500	107
H20	H23	4.474866	0.450919	0.170100	109
C2	H27	4.477266	0.368937	0.065300	107
H15	H28	4.478862	0.450919	0.169800	109
B13	H19	4.500862	0.408645	−0.028600	107
B12	H27	4.508545	0.408089	−0.028400	107
C6	B13	4.515947	0.112274	0.012700	108
C7	B12	4.515947	0.112172	0.012700	108
H16	H30	4.530683	0.222411	0.049200	108
H24	H31	4.530684	0.222309	0.049200	108
C11	H32	4.548673	0.110747	0.019700	108
C10	H33	4.548773	0.110747	0.019600	108
C5	H34	4.605123	0.110951	0.020400	108
C4	H35	4.605323	0.110951	0.020200	108

B13	H33	4.624481	0.128052	0.021100	108
B12	H32	4.624481	0.128052	0.021100	108
C5	H30	4.624621	0.110849	0.020200	108
C4	H31	4.624621	0.110849	0.020200	108
C5	C18	4.625908	0.134261	0.018200	108
C4	C26	4.628435	0.134159	0.018100	108
H33	H34	4.680210	0.176300	0.020800	108
H32	H35	4.680210	0.176300	0.020800	108
C3	C22	4.706464	0.152074	0.023900	108
C3	C14	4.706506	0.152074	0.023900	108
C7	H25	4.716606	0.225465	0.021700	108
C6	H17	4.716624	0.225465	0.021700	108
C9	H16	4.721126	0.395198	0.067900	109
C8	H24	4.721165	0.394838	0.067800	109
H21	H23	4.736033	0.513428	0.101700	108
C2	H28	4.756371	0.218329	0.070100	109
C2	H20	4.756498	0.218569	0.070400	109
H15	H29	4.770209	0.513428	0.101700	108
H25	H31	4.784335	0.296578	0.037400	109
H17	H30	4.784345	0.296578	0.037400	109
C7	H34	4.786968	0.152064	0.020600	109
C6	H35	4.787268	0.152064	0.020300	109
C8	C9	4.813467	0.079207	0.015700	109
B12	H28	4.824184	0.332527	0.076200	109
C14	H31	4.824238	0.295020	0.021000	109
C22	H30	4.824293	0.295140	0.020900	109
B13	H20	4.825346	0.333006	0.076400	109
C6	C7	4.834460	0.080885	0.016200	109
C5	H19	4.902966	0.352397	0.029400	108
C4	H27	4.909290	0.351786	0.029300	108
C26	H33	4.931164	0.233610	0.015200	110
C18	H32	4.933350	0.233610	0.015100	110
C10	H24	5.008451	0.322941	0.071500	109
C11	H16	5.008607	0.323300	0.071400	109
C7	C8	5.022761	0.083282	0.017100	109
C6	C9	5.022861	0.083282	0.017000	109
C9	H27	5.025948	0.406367	0.115000	110
C8	H19	5.028844	0.407003	0.115400	110
C8	H20	5.033264	0.509515	0.088100	109
C10	H21	5.034215	0.310249	−0.049800	110
C9	H28	5.034305	0.508557	0.087700	109
C11	H29	5.035661	0.310249	−0.049600	110
C8	C14	5.077137	0.177707	0.027000	109
C9	C22	5.077212	0.177707	0.026900	109
C7	H15	5.093242	0.402293	0.083700	110
C6	H23	5.093392	0.401783	0.083500	110
B13	H21	5.098778	0.361885	0.032500	109
B12	H29	5.111863	0.361765	0.032500	109
C5	H21	5.112796	0.280881	0.011500	109
C7	H17	5.122254	0.365501	−0.028100	110
C6	H25	5.122318	0.365119	−0.028200	110
C4	H29	5.125665	0.280761	0.011500	109
C10	B13	5.127696	0.108848	0.016600	110
C11	B12	5.127896	0.108848	0.016400	110
C3	H23	5.136138	0.429110	0.079100	109
C3	H15	5.136282	0.429110	0.079000	109
C8	H16	5.140580	0.181302	0.066100	109
C9	H24	5.140756	0.180823	0.065900	109
C3	C18	5.144424	0.120815	0.020000	110
C3	C26	5.145270	0.120815	0.020100	110
B12	H31	5.156859	0.198855	0.019100	110
B13	H30	5.156959	0.198855	0.019000	110
C3	H21	5.168350	0.286188	−0.027900	110
C3	H29	5.175118	0.286188	−0.027400	110
C10	H16	5.212976	0.209702	0.070700	109

C11	H24	5.213138	0.209103	0.070500	109
C10	H31	5.253209	0.127053	0.024900	110
C11	H30	5.253409	0.127053	0.024700	110
C4	H28	5.268753	0.216933	0.075100	110
C5	H20	5.269351	0.217060	0.075400	110
C10	C18	5.273689	0.141566	0.015800	110
C11	C26	5.273730	0.141566	0.015600	110
C9	H23	5.275270	0.441332	0.056500	109
C8	H15	5.275298	0.441332	0.056500	109
C5	H32	5.316079	0.127562	0.026600	110
C4	H33	5.316179	0.127562	0.026500	110
H17	H31	5.326379	0.422407	−0.023100	110
H25	H30	5.326444	0.422153	−0.023200	110
C8	B13	5.354751	0.130491	0.018100	110
C9	B12	5.354751	0.130491	0.018100	110
C10	C14	5.426171	0.197709	0.027600	110
C11	C22	5.426335	0.197709	0.027400	110
B12	H34	5.442544	0.139911	0.026200	110
B13	H35	5.442744	0.139911	0.026000	110
H15	H31	5.484458	0.434830	0.089500	111
H23	H30	5.484510	0.434309	0.089400	111
H20	H32	5.505701	0.638958	0.096100	110
H28	H33	5.507052	0.637812	0.095700	110
C8	C22	5.553405	0.255634	0.025500	110
C9	C14	5.553454	0.255634	0.025500	110
H27	H33	5.585168	0.436654	0.132500	111
H19	H32	5.589843	0.437044	0.132900	111
H16	H33	5.612467	0.463655	0.081600	110
H24	H32	5.612506	0.463273	0.081500	110
C3	H19	5.615293	0.446723	0.091700	110
C3	H27	5.617659	0.445832	0.091500	110
C3	H17	5.643681	0.335965	−0.005200	110
C3	H25	5.643750	0.335711	−0.005300	110
C10	C22	5.657091	0.228645	0.026900	110
C11	C14	5.657238	0.228645	0.026800	110
C18	C26	5.700934	0.335329	0.029200	110
C10	H15	5.724206	0.490390	0.070600	110
C11	H23	5.724368	0.490390	0.070400	110
C9	H32	5.758138	0.137692	0.028000	111
C8	H33	5.758238	0.137692	0.027900	111
C6	H31	5.799270	0.137171	0.027900	111
C7	H30	5.799270	0.137171	0.027900	111
H19	C26	5.805501	0.474166	−0.038400	109
C18	H27	5.813022	0.473806	−0.038000	109
H31	H34	5.830696	0.194228	0.034300	111
H30	H35	5.830996	0.194228	0.034000	111
C11	H27	5.833042	0.446945	0.110500	111
C10	H19	5.833126	0.447726	0.111000	111
C3	H20	5.881043	0.326709	0.087100	111
C3	H28	5.881043	0.326188	0.086900	111
C14	H32	5.946716	0.249200	0.040800	111
C22	H33	5.946794	0.249200	0.040700	111
H19	H28	5.956815	0.694591	−0.014400	110
H20	H27	5.971123	0.694973	−0.013800	110
C10	H20	5.984131	0.463098	0.089900	111
C11	H28	5.984977	0.462186	0.089300	111
H21	H34	5.991652	0.346118	−0.039500	111
H29	H35	5.993116	0.346118	−0.039300	111
C7	C18	5.996506	0.174297	0.027700	111
C6	C26	5.999301	0.174297	0.027600	111
C8	H17	6.005875	0.344555	0.022600	111
C9	H25	6.006053	0.344425	0.022400	111
C18	H28	6.012713	0.521327	0.085700	111
H19	H27	6.015056	0.578297	−0.118400	109
H20	C26	6.018960	0.521978	0.085900	111

H24	H34	6.038278	0.356930	0.090200	111
H16	H35	6.038434	0.357452	0.090100	111
B13	H34	6.050152	0.155017	0.030200	111
B12	H35	6.050252	0.155017	0.030100	111
C7	H32	6.061090	0.133263	0.031000	111
C6	H33	6.061290	0.133263	0.030800	111
H23	H33	6.063075	0.522499	0.058500	111
H15	H32	6.063097	0.522499	0.058500	111
C8	H31	6.071219	0.132481	0.030500	111
C9	H30	6.071419	0.132481	0.030300	111
H24	H33	6.098769	0.251154	0.082400	111
H16	H32	6.098789	0.251545	0.082400	111
C8	H23	6.108096	0.472868	0.090500	111
C9	H15	6.108149	0.473259	0.090500	111
C10	H23	6.128624	0.494362	0.086900	111
C11	H15	6.128874	0.494492	0.086700	111
H16	H34	6.204725	0.264832	0.090400	111
H24	H35	6.204885	0.264181	0.090200	111
C7	H19	6.238932	0.467397	0.035300	111
C6	H27	6.245901	0.466615	0.035300	111
C18	H34	6.298030	0.138353	0.030900	112
C26	H35	6.298054	0.138353	0.030700	112
H20	H28	6.305609	0.550303	0.171700	112
C9	H17	6.333061	0.294651	−0.022300	112
C8	H25	6.333125	0.294351	−0.022400	112
C10	H17	6.390142	0.279212	0.009800	112
C11	H25	6.390314	0.279112	0.009600	112
B12	H33	6.395556	0.131034	0.032800	112
B13	H32	6.395556	0.131034	0.032800	112
C11	C18	6.427175	0.101058	0.028400	112
C10	C26	6.428540	0.101058	0.028600	112
C7	H21	6.438845	0.243822	0.018600	112
C6	H29	6.453604	0.243621	0.018600	112
C14	H34	6.473138	0.190385	0.042800	112
C22	H35	6.473301	0.190385	0.042600	112
C22	H32	6.508757	0.235801	0.039400	112
C14	H33	6.508806	0.235801	0.039400	112
C11	H21	6.515933	0.234297	−0.013000	112
H21	C26	6.516038	0.413596	0.066200	111
C18	H29	6.524036	0.413596	0.066100	111
C10	H29	6.525988	0.234197	−0.012600	112
C10	H25	6.549347	0.287333	−0.013300	112
C11	H17	6.549582	0.287633	−0.013500	112
C18	H31	6.633280	0.184470	0.035300	112
C26	H30	6.636482	0.184470	0.035200	112
C6	H28	6.646864	0.177051	0.089000	112
C7	H20	6.647528	0.177252	0.089300	112
H32	H33	6.651372	0.139857	0.040100	112
H19	H29	6.663047	0.531097	0.025500	111
C22	H34	6.663685	0.207028	0.042400	112
C14	H35	6.663832	0.207028	0.042300	112
H21	H27	6.670369	0.530706	0.026000	111
H30	H31	6.720140	0.137730	0.039400	113
H15	H34	6.751093	0.421976	0.083200	112
H23	H35	6.751252	0.421976	0.083000	112
C9	C18	6.778666	0.117352	0.033000	113
C8	C26	6.780969	0.117352	0.033000	113
H19	H31	6.798359	0.379167	0.018500	112
H27	H30	6.806477	0.378666	0.018600	112
C11	H19	6.828323	0.368719	0.086100	113
C10	H27	6.832098	0.367916	0.086100	113
H27	H35	6.846808	0.360911	0.129200	114
H19	H34	6.846891	0.361511	0.129800	114
H17	H32	6.851507	0.296441	0.041500	113
H25	H33	6.851588	0.296441	0.041400	113

H21	H28	6.877447	0.447240	0.117200	112
H20	H29	6.897604	0.447441	0.117200	112
H20	H34	7.003073	0.386125	0.105800	114
H28	H35	7.003969	0.385425	0.105200	114
C9	H21	7.049132	0.240726	0.007800	113
H15	H33	7.058652	0.392129	0.105400	114
H23	H32	7.058698	0.391829	0.105300	114
C8	H29	7.062608	0.240626	0.008000	113
C9	H19	7.087322	0.369823	0.063900	113
H23	H34	7.089131	0.418209	0.098500	113
H15	H35	7.089282	0.418209	0.098400	113
C8	H27	7.093131	0.369120	0.063900	113
H31	H32	7.114763	0.126174	0.045900	114
H30	H33	7.114963	0.126174	0.045700	114
C10	H28	7.162856	0.220529	0.096300	114
C11	H20	7.163171	0.220929	0.096400	114
H21	H31	7.176548	0.277668	0.038700	113
H29	H30	7.192923	0.277568	0.038700	113
H28	H30	7.226351	0.238139	0.098100	114
H20	H31	7.227219	0.238239	0.098400	114
H17	H33	7.246838	0.323489	−0.012200	114
H25	H32	7.246901	0.323289	−0.012300	114
H21	H35	7.255817	0.259852	−0.007900	114
H29	H34	7.264873	0.259752	−0.007500	114
C18	H35	7.271011	0.134879	0.042300	114
C26	H34	7.272125	0.134879	0.042500	114
H21	H29	7.274628	0.330271	0.092900	113
H17	H34	7.446509	0.311582	0.021800	114
H25	H35	7.446680	0.311482	0.021600	114
C8	H28	7.483279	0.177003	0.098400	114
C9	H20	7.483820	0.177303	0.098600	114
H25	H34	7.580403	0.313583	0.002600	114
H17	H35	7.580538	0.313783	0.002500	114
H19	H35	7.694455	0.385025	0.109900	114
H27	H34	7.697660	0.384324	0.109800	114
C18	H33	7.825362	0.142283	0.050000	114
C26	H32	7.827859	0.142283	0.050000	114
H28	H34	8.012762	0.270658	0.113200	114
H20	H35	8.012847	0.271058	0.113400	114
H21	H33	8.102717	0.258051	0.026200	114
H19	H33	8.106856	0.383724	0.075000	114
H27	H32	8.113315	0.383024	0.074900	114
H29	H32	8.117164	0.257951	0.026500	114
H28	H32	8.524506	0.193513	0.117700	114
H20	H33	8.525116	0.193713	0.117900	114

Quantum-chemical calculations

Optimization of the geometrical structure has been performed using the PBE0[1] density functional with the dispersion correction D3 incorporating the Becke-Johnson damping (BJ)[2] with the def2TZVPP [3] basis set. All quantum-chemical calculation were performed using the Gaussian16/D.01[4] program suite.

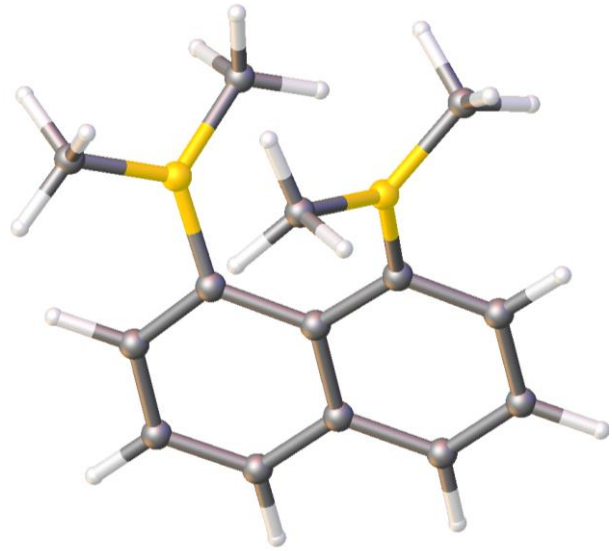
For the ion pair of [1-H][3-H] the starting geometry taken from a CREST calculation.[5]

The energy for the experimentally not observed reaction of **1** and **3** with molecular hydrogen to form the ion pair [**1**-H][**3**-H] was calculated using the sum of electronic and thermal Energies given in the thermochemistry output of the optimization and subsequent frequency calculations.

	1	**3**	H_2	[**1**-H][**3**-H]
Energy/hartree	–593.211240	–652.936083	–1.154057	–1247.320159

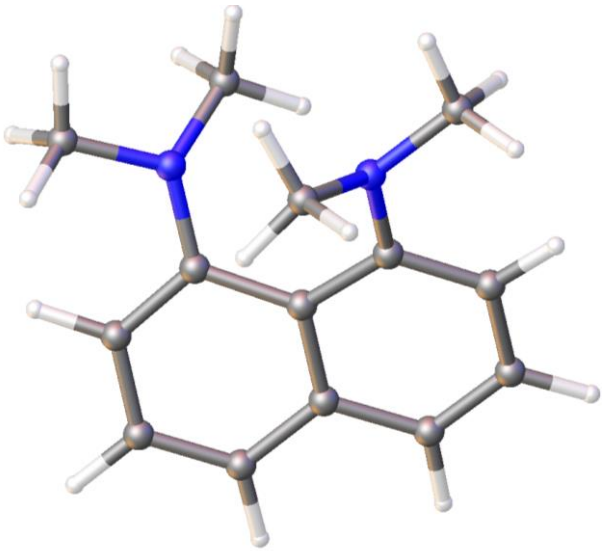
In the following the optimized minimum structures of the respective compounds are listed.

Table S8. Cartesian coordinates of the optimized structure of **1** along with a depiction of the structure.



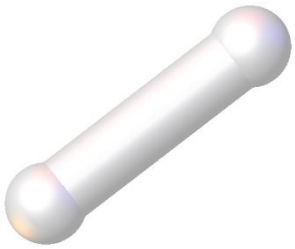
Atom Symbol	*X*	*Y*	*Z*
C	−0.689928	−0.000258	−0.000092
C	−2.126859	−0.001196	0.000235
C	0.005827	−1.257871	0.012289
C	0.004254	1.258257	−0.012846
C	−0.744433	−2.431132	−0.085098
C	−0.747571	2.430545	0.084229
C	−2.154797	−2.428813	−0.102933
C	−2.157916	2.426405	0.102716
C	−2.832704	−1.231901	−0.043878
C	−2.834292	1.228584	0.044537
B	1.517191	−1.463619	0.362497
B	1.515512	1.465760	−0.362934
C	2.159163	−0.724999	1.601452
H	2.101996	−1.466067	2.422490
H	1.639204	0.171239	1.960826
H	3.231199	−0.508492	1.482041
C	2.379859	−2.568864	−0.358584
H	3.159835	−2.055069	−0.947099
H	2.931971	−3.197670	0.357963
H	1.830150	−3.216957	−1.054033
C	2.158496	0.726716	−1.601007
H	2.097590	1.466003	−2.423406
H	1.640620	−0.171790	−1.957733
H	3.231381	0.513842	−1.482846
C	2.376448	2.571918	0.358614
H	3.149944	2.057437	0.955158
H	2.936052	3.196066	−0.356087
H	1.823893	3.224218	1.047902
H	−0.225415	−3.391735	−0.105728
H	−0.229772	3.391806	0.104100
H	−2.700253	−3.372236	−0.151853
H	−2.704587	3.369132	0.151468
H	−3.924527	−1.208435	−0.035221
H	−3.926089	1.203670	0.036429

Table S9. Cartesian coordinates of the optimized structure of **3** along with a depiction of the structure.



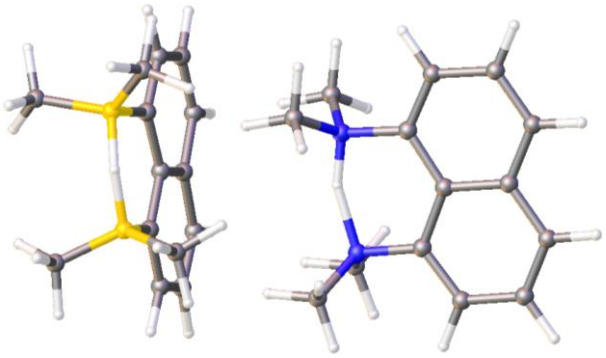
Atom Symbol	*X*	*Y*	*Z*
C	−0.594453	0.000101	0.000010
C	−2.035603	0.000341	0.000020
C	0.069432	−1.287023	0.013272
C	0.069865	1.286996	−0.013277
C	−0.675118	−2.434160	−0.261632
C	−0.674309	2.434392	0.261570
C	−2.072586	−2.387496	−0.420996
C	−2.071788	2.388195	0.420977
C	−2.748683	−1.204454	−0.233848
C	−2.748283	1.205373	0.233885
N	1.437085	−1.386304	0.314932
N	1.437552	1.385831	−0.314943
C	1.884701	−0.814624	1.579213
H	1.830872	−1.567108	2.391643
H	1.259279	0.036611	1.857698
H	2.925340	−0.468077	1.493805
C	2.120969	−2.623125	0.002538
H	3.203715	−2.454009	0.089290
H	1.858724	−3.460207	0.683314
H	1.900989	−2.931681	−1.027693
C	1.884962	0.814012	−1.579224
H	1.831052	1.566397	−2.391742
H	1.259493	−0.037256	−1.857491
H	2.925605	0.467453	−1.493908
C	2.121889	2.622390	−0.002508
H	3.204580	2.452807	−0.089061
H	1.860132	3.459549	−0.683378
H	1.901864	2.931100	1.027666
H	−0.180580	−3.403482	−0.276723
H	−0.179441	3.403548	0.276623
H	−2.617328	−3.310616	−0.624402
H	−2.616217	3.311505	0.624363
H	−3.838449	−1.167301	−0.265038
H	−3.838059	1.168581	0.265099

Table S10. Cartesian coordinates of the optimized structure of H_2 along with a depiction of the structure.



Atom Symbol	*X*	*Y*	*Z*
H	0.000000	0.000000	0.375428
H	0.000000	0.000000	−0.375428

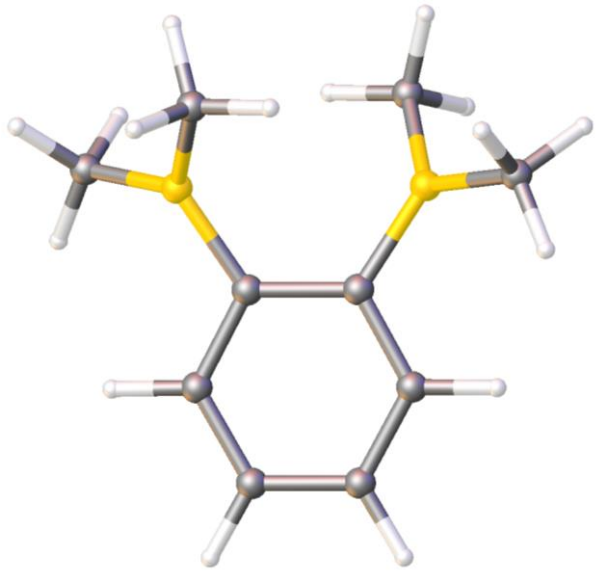
Table S11. Cartesian coordinates of the optimized structure of [**1**-H][**3**-H] along with a depiction of the structure.



Atom Symbol	*X*	*Y*	*Z*
C	−2.455783	2.563550	0.020446
C	−2.173710	2.939315	1.354152
C	−2.115054	1.987204	2.353655
C	−2.363271	0.621764	2.050721
C	−2.352536	−0.384261	3.054078
C	−2.634758	−1.696569	2.723392
C	−2.944602	−2.050089	1.390094
C	−2.990786	−1.108963	0.363506
C	−2.669572	0.251005	0.691956
C	−2.701989	1.241638	−0.345127
B	−3.040924	0.850247	−1.862963
C	−4.384470	1.540457	−2.436180
H	−5.259962	1.385213	−1.788600
H	−4.644724	1.176305	−3.442801
H	−4.241243	2.632130	−2.520946
C	−1.779101	0.928015	−2.886135
H	−0.897515	0.353592	−2.558660
H	−2.046175	0.567698	−3.891938
H	−1.452739	1.977017	−3.002419
H	−3.313807	−0.452526	−1.894256
B	−3.554648	−1.487574	−1.091067
C	−5.168943	−1.608461	−1.072631
H	−5.589344	−1.700683	−2.086634
H	−5.465241	−2.514065	−0.515254
H	−5.662189	−0.756740	−0.580747
C	−2.818076	−2.692082	−1.892782
H	−3.371645	−2.966186	−2.804323
H	−1.786187	−2.471058	−2.209718
H	−2.773394	−3.601179	−1.266816
H	−3.195407	−3.091581	1.170096
H	−2.635472	−2.464337	3.500887
H	−2.137578	−0.100949	4.087457
H	−1.909463	2.272300	3.388667
H	−2.009394	3.992363	1.596044
H	−2.507060	3.345740	−0.742690
C	3.976967	2.173435	−0.312898
C	5.334093	1.881739	−0.558551
C	5.761015	0.573133	−0.590674
C	4.851523	−0.494270	−0.382898
C	5.292608	−1.841627	−0.421543
C	4.414897	−2.884428	−0.227028
C	3.051395	−2.618511	0.013567
C	2.592536	−1.320742	0.057965
C	3.461221	−0.204895	−0.133293
C	3.055360	1.166856	−0.102529
N	1.658532	1.480537	0.155944
C	1.459746	2.159154	1.452510
H	0.381820	2.235134	1.649014

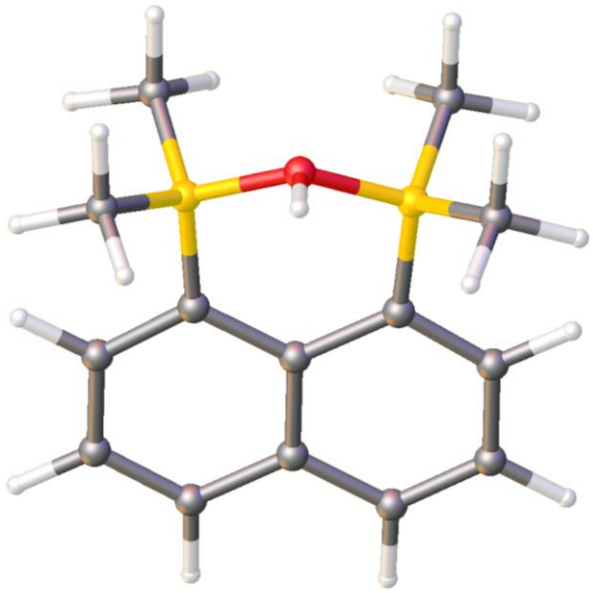
H	1.899247	3.170913	1.451844
H	1.935403	1.572902	2.248763
C	1.012255	2.217957	−0.948911
H	1.156349	1.672978	−1.888558
H	−0.063375	2.284325	−0.742350
H	1.424705	3.235118	−1.055803
H	1.137958	0.073952	0.255460
N	1.166022	−1.060215	0.304077
C	0.274717	−1.610691	−0.755955
H	−0.749334	−1.279335	−0.550816
H	0.308378	−2.705918	−0.744669
H	0.607602	−1.236959	−1.729430
C	0.723571	−1.476258	1.664876
H	1.393112	−1.025885	2.405638
H	0.760336	−2.568599	1.750498
H	−0.305064	−1.132969	1.823787
H	2.356448	−3.445516	0.159986
H	4.763253	−3.916228	−0.260767
H	6.348896	−2.035944	−0.612298
H	6.808450	0.334365	−0.779400
H	6.039199	2.696707	−0.721964
H	3.645615	3.212041	−0.288980

Table S12. Cartesian coordinates of the optimized structure of **2** along with a depiction of the structure.



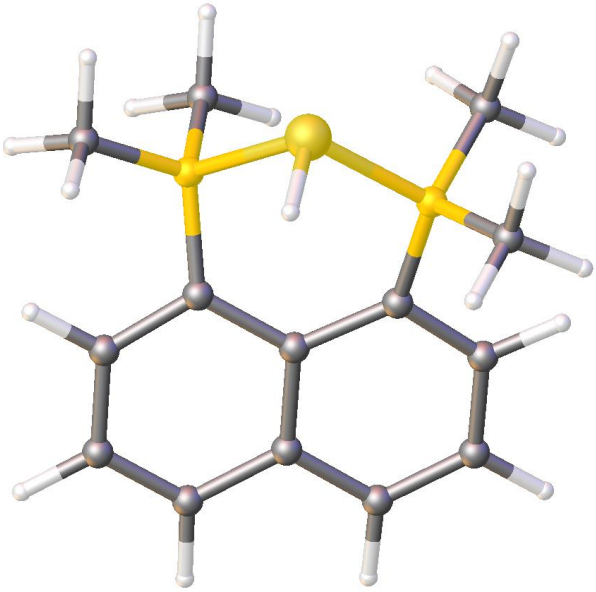
Atom	*X*	*Y*	*Z*
C	2.753567	-0.644759	-0.217050
C	2.744810	0.678462	0.220933
C	1.542812	-1.304558	-0.441626
C	1.525411	1.322675	0.443943
C	0.302544	-0.677063	-0.223799
C	0.293561	0.679328	0.224565
B	-0.995350	-1.547504	-0.350922
B	-1.015585	1.532973	0.350116
C	-2.096576	-1.489316	0.770882
H	-3.115593	-1.687904	0.407760
H	-1.859654	-2.316371	1.467963
H	-2.097435	-0.575120	1.381561
C	-1.176281	-2.551751	-1.548019
H	-1.745792	-3.455739	-1.286030
H	-1.790808	-2.024298	-2.302559
H	-0.248642	-2.837123	-2.062839
C	-2.115009	1.459984	-0.772566
H	-3.136829	1.645416	-0.410371
H	-1.888307	2.289771	-1.469798
H	-2.103414	0.545598	-1.382854
C	-1.210569	2.535313	1.546608
H	-1.791639	3.431664	1.283772
H	-1.818722	2.000191	2.300913
H	-0.287150	2.833021	2.062032
H	3.699061	-1.162184	-0.387573
H	3.683382	1.207957	0.392633
H	1.564103	-2.343114	-0.779519
H	1.532965	2.361426	0.781828

Table S13. Cartesian coordinates of the optimized structure of [**1**-OH]$^-$ along with a depiction of the structure.



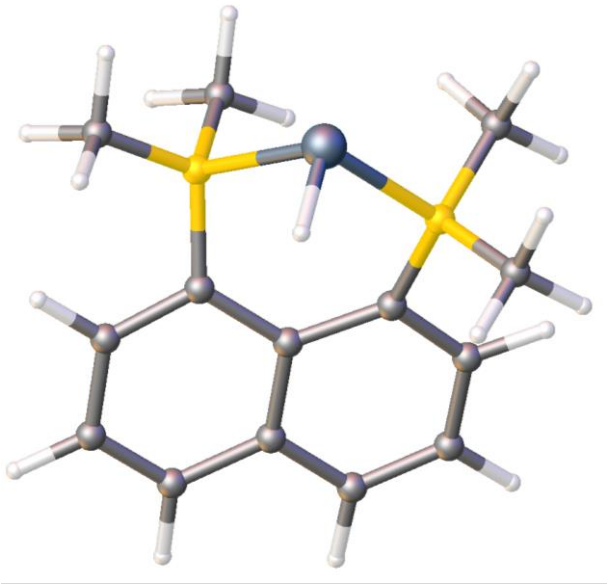
Atom Symbol	*X*	*Y*	*Z*
C	−0.889630	2.424291	−0.006642
C	−2.300490	2.425217	0.015416
C	−2.987720	1.230692	0.009144
C	−2.281105	0.000423	−0.010393
C	−0.833408	0.000098	−0.033976
C	−0.129964	1.257414	−0.036900
C	−0.130526	−1.257543	−0.037237
C	−0.890721	−2.424089	−0.007800
C	−2.301594	−2.424380	0.013986
C	−2.988277	−1.229544	0.008393
H	−0.372200	3.388091	0.000603
H	−2.844934	3.373661	0.035682
H	−4.081324	1.207841	0.026099
B	1.484131	1.396600	−0.024977
B	1.483514	−1.397225	−0.024026
H	−0.373741	−3.388127	−0.000882
H	−2.846474	−3.372587	0.033615
H	−4.081871	−1.206206	0.025326
C	2.039158	−1.803095	1.451780
C	2.032307	−2.416079	−1.179351
C	2.032116	2.414112	−1.181894
C	2.041180	1.803999	1.449876
H	1.712491	2.119656	−2.199641
H	3.135366	2.470044	−1.180033
H	1.663245	3.441245	−1.032549
H	1.700881	−1.118267	2.244450
H	3.142613	−1.822811	1.478232
H	1.684168	−2.810440	1.727447
H	1.713592	−2.122711	−2.197697
H	1.663227	−3.443020	−1.029196
H	3.135545	−2.472122	−1.176495
H	1.703812	1.119892	2.243552
H	1.686349	2.811569	1.724933
H	3.144659	1.823896	1.475192
O	2.122878	−0.000579	−0.412967
H	2.225377	−0.000933	−1.376308

Table S14. Cartesian coordinates of the optimized structure of [**1**-SH]$^-$ along with a depiction of the structure.



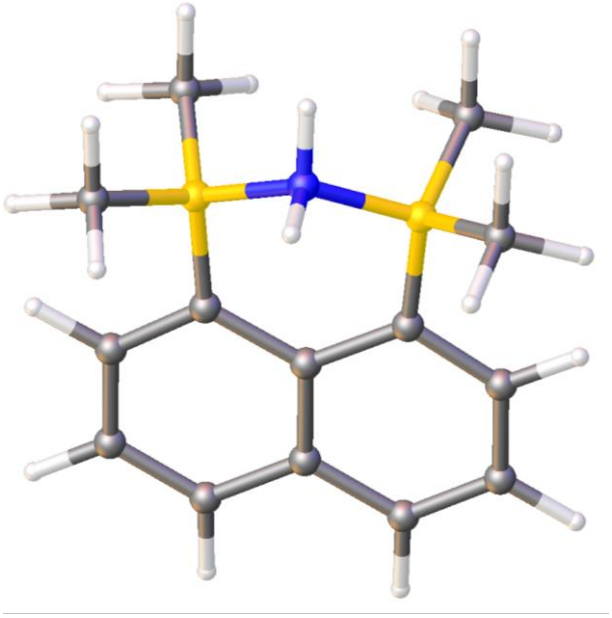
Atom Symbol	*X*	*Y*	*Z*
C	0.860158	−2.442717	0.277797
C	2.263816	−2.532415	0.346071
C	3.022170	−1.397901	0.164859
C	2.391623	−0.142021	−0.022971
C	0.945110	−0.034438	−0.013277
C	0.167122	−1.248818	0.070178
C	0.356272	1.287337	−0.075838
C	1.210828	2.369338	−0.274692
C	2.614824	2.248351	−0.360934
C	3.197458	1.012483	−0.210380
H	0.284972	−3.369128	0.359080
H	2.742943	−3.501827	0.508468
H	4.115125	−1.439556	0.164730
B	−1.429460	−1.462282	−0.162039
B	−1.189439	1.634059	0.255178
H	0.779129	3.370276	−0.338256
H	3.231394	3.137902	−0.517507
H	4.284532	0.891876	−0.225868
C	−1.477357	1.510452	1.857190
C	−1.729734	3.053708	−0.336437
C	−1.707044	−2.416585	−1.462465
C	−2.210356	−2.025400	1.156136
H	−1.112364	0.570574	2.296525
H	−2.547961	1.607052	2.107988
H	−0.948844	2.331440	2.371753
H	−1.206739	−2.051984	−2.375848
H	−2.784660	−2.504548	−1.684624
H	−1.332426	−3.439078	−1.284156
H	−2.133983	−1.368036	2.035321
H	−1.783639	−2.999957	1.449752
H	−3.283224	−2.191018	0.957853
H	−1.536071	3.185456	−1.415189
H	−1.260400	3.909337	0.180414
H	−2.816705	3.158888	−0.183278
S	−2.322762	0.249680	−0.605805
H	−1.861733	0.400332	−1.871388

Table S15. Cartesian coordinates of the optimized structure of [**1**-SeH]$^-$ along with a depiction of the structure.



Atom Symbol	*X*	*Y*	*Z*
C	1.338816	−2.381709	0.365601
C	2.746563	−2.374221	0.374207
C	3.414103	−1.199782	0.111335
C	2.689013	0.003008	−0.082102
C	1.241608	0.017705	0.013028
C	0.553741	−1.246308	0.150830
C	0.570847	1.302923	−0.021452
C	1.339261	2.426987	−0.317691
C	2.737046	2.388402	−0.512924
C	3.405609	1.197626	−0.361312
H	0.834968	−3.343969	0.490826
H	3.297890	−3.302670	0.546012
H	4.505535	−1.167908	0.049158
B	−1.016320	−1.619922	−0.066506
B	−0.942667	1.580469	0.469773
H	0.844424	3.398891	−0.363723
H	3.282648	3.307749	−0.743016
H	4.494816	1.143034	−0.445099
C	−1.109161	1.286075	2.063177
C	−1.574830	3.019934	0.054954
C	−1.204319	−2.566216	−1.384997
C	−1.738118	−2.266999	1.243639
H	−0.688921	0.320444	2.379037
H	−2.158446	1.327645	2.403191
H	−0.562256	2.069369	2.617366
H	−0.754667	−2.131646	−2.293261
H	−2.267652	−2.766455	−1.601690
H	−0.718335	−3.545629	−1.229837
H	−1.735548	−1.611631	2.127888
H	−1.212272	−3.193002	1.535854
H	−2.785954	−2.546967	1.040713
H	−1.492479	3.250146	−1.021099
H	−1.078876	3.844233	0.599282
H	−2.643690	3.074502	0.319379
Se	−2.180507	0.119540	−0.492131
H	−1.690076	0.362220	−1.872625

Table S16. Cartesian coordinates of the optimized structure of [**1**-NH_2]$^-$ along with a depiction of the structure.

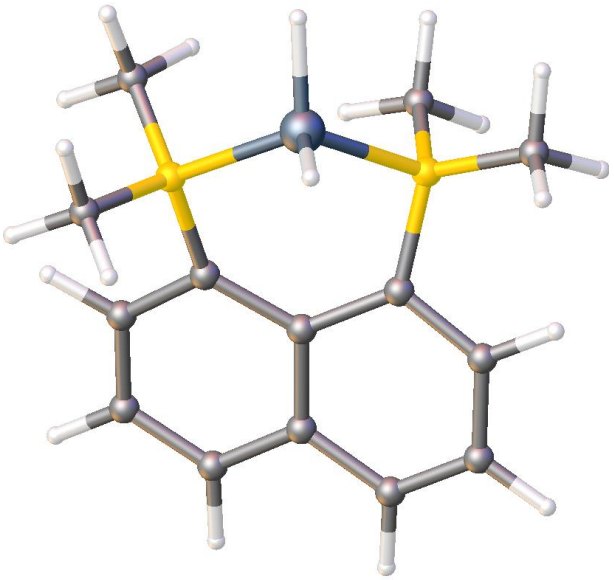


Atom Symbol	*X*	*Y*	*Z*
C	−0.024870	0.904460	2.425121
C	0.009834	2.314902	2.424483
C	0.012691	2.999704	1.228901
C	−0.010715	2.290765	−0.000000
C	−0.044728	0.842546	−0.000000
C	−0.054690	0.141080	1.260420
C	−0.054690	0.141080	−1.260420
C	−0.024870	0.904460	−2.425121
C	0.009834	2.314902	−2.424483
C	0.012691	2.999704	−1.228901
H	−0.027778	0.389032	3.389584
H	0.031892	2.860530	3.372298
H	0.038315	4.093157	1.203408
B	−0.041268	−1.475482	1.402627
B	−0.041268	−1.475482	−1.402627
H	−0.027778	0.389032	−3.389584
H	0.031892	2.860530	−3.372298
H	0.038315	4.093157	−1.203408
C	−1.113673	−2.012212	−2.526623
C	1.460786	−2.019089	−1.763094
C	1.460786	−2.019089	1.763094
C	−1.113673	−2.012212	2.526623
H	−2.148230	−1.676668	−2.326038
H	−1.131838	−3.118032	−2.568788
H	−0.867629	−1.671284	−3.545674
H	2.239163	−1.661592	1.072443
H	1.511574	−3.125045	1.769596
H	1.750260	−1.683756	2.773161
H	−2.148230	−1.676668	2.326038
H	−0.867629	−1.671284	3.545674
H	−1.131838	−3.118032	2.568788
H	2.239163	−1.661592	−1.072443
H	1.750260	−1.683756	−2.773161
H	1.511574	−3.125045	−1.769596
N	−0.522440	−2.100122	−0.000000
H	−1.546732	−2.057379	−0.000000
H	−0.306247	−3.102059	−0.000000

Table S17. Cartesian coordinates of the optimized structure of [**1**-PH_2]$^-$ along with a depiction of the structure.

Atom Symbol	*X*	*Y*	*Z*
C	2.112047	0.585510	1.428317
C	1.986650	−0.819330	1.477352
C	0.949416	−1.427152	0.811685
C	−0.024159	−0.646507	0.133523
C	0.049552	0.803587	0.148060
C	1.217242	1.416897	0.758573
C	−1.044374	1.546183	−0.445160
C	−2.025033	0.818207	−1.119738
C	−2.042423	−0.587023	−1.205332
C	−1.068870	−1.311790	−0.557017
H	2.980535	1.037972	1.910865
H	2.728867	−1.416020	2.014980
H	0.849752	−2.516201	0.789352
B	1.693926	2.970026	0.564243
B	−1.388945	3.149717	−0.352923
H	−2.848183	1.368024	−1.584110
H	−2.842443	−1.093035	−1.752765
H	−1.079825	−2.405477	−0.557640
C	−1.340907	3.885895	−1.817039
C	−2.837449	3.400872	0.374821
C	2.790367	3.508456	1.645915
C	2.228446	3.180594	−0.973276
H	−0.365761	3.821121	−2.323699
H	−1.606029	4.955490	−1.746808
H	−2.080617	3.417569	−2.490261
H	2.492367	3.347770	2.696298
H	2.970205	4.590258	1.521846
H	3.772213	3.018966	1.510575
H	1.528141	2.815434	−1.738669
H	3.165952	2.610355	−1.097360
H	2.458546	4.235381	−1.204705
H	−2.908784	2.925379	1.367261
H	−3.666135	2.995442	−0.232427
H	−3.043999	4.477350	0.510562
P	0.017225	3.950446	0.752223
H	−0.363619	3.996582	2.125496
H	0.127616	5.356991	0.530281

Table S18. Cartesian coordinates of the optimized structure of [**1**-AsH_2]$^-$ along with a depiction of the structure.



Atom Symbol	*X*	*Y*	*Z*
C	2.059860	0.593110	1.527318
C	1.907419	−0.807828	1.599699
C	0.901333	−1.410829	0.884952
C	−0.024382	−0.627115	0.145539
C	0.058185	0.823192	0.152564
C	1.215701	1.427310	0.796770
C	−1.015124	1.563665	−0.483289
C	−1.953082	0.831744	−1.214069
C	−1.962526	−0.572620	−1.305730
C	−1.029924	−1.295025	−0.598385
H	2.916119	1.039005	2.036425
H	2.610415	−1.405303	2.186700
H	0.789664	−2.498742	0.867830
B	1.763217	2.948515	0.566189
B	−1.439260	3.147741	−0.371682
H	−2.756955	1.378769	−1.713937
H	−2.729775	−1.078665	−1.897992
H	−1.043202	−2.388579	−0.591608
C	−1.414304	3.923203	−1.810922
C	−2.888258	3.311465	0.370536
C	2.917347	3.457004	1.593283
C	2.216519	3.143706	−0.994379
H	−0.431686	3.921128	−2.308181
H	−1.733880	4.975547	−1.716483
H	−2.121106	3.438570	−2.508326
H	2.653447	3.335899	2.657771
H	3.141765	4.525382	1.435062
H	3.869354	2.917189	1.433409
H	1.456935	2.821079	−1.721594
H	3.113809	2.524892	−1.174827
H	2.491569	4.185592	−1.233787
H	−2.925896	2.823402	1.358446
H	−3.696492	2.862943	−0.234786
H	−3.153985	4.372918	0.517432
As	0.020979	4.051226	0.806724
H	−0.381084	4.149581	2.278183
H	0.138792	5.554870	0.538448

Natural localized molecular orbitals (NLMO) and second order perturbation energies were obtained by NBO analysis with NBO 7.0[6] based on PBE0(D3BJ)/def2-TZVPP densities obtained from Gaussian16. Selected output is listed below.

Table S19. Second order perturbation analysis of the Fock matrix. In NBO-basis for **1**. Threshold for printing the donor acceptor interactions in 0.50 kcal/mol. E(2) is the energy of the donor-acceptor interaction in kcal/mol, E(NL) – E(L) is the energy difference between the donor and acceptor in atomic units and F(L,NL) is the overlap between the donor and acceptor natural orbitals in atomic units.

Donor (L) NBO	Acceptor (NL) NBO	E(2) / kcal/mol	E(NL) – E(L) / a.u	F(L,NL) / a.u.
17.BD(1)C1-C2	61.BD*(1)C1-C3	0.67	0.95	0.023
17.BD(1)C1-C2	62.BD*(1)C1-C4	0.67	0.95	0.023
17.BD(1)C1-C2	63.BD*(1)C2-C9	0.72	0.96	0.023
17.BD(1)C1-C2	64.BD*(1)C2-C10	0.72	0.96	0.023
17.BD(1)C1-C2	67.BD*(1)C3-B11	2.53	0.90	0.043
17.BD(1)C1-C2	70.BD*(1)C4-B12	2.53	0.90	0.043
17.BD(1)C1-C2	81.BD*(1)C9-H33	2.19	0.85	0.039
17.BD(1)C1-C2	82.BD*(1)C10-H34	2.19	0.85	0.039
17.BD(1)C1-C2	151.RY(1)C3	0.75	1.88	0.034
17.BD(1)C1-C2	177.RY(1)C4	0.75	1.88	0.034
17.BD(1)C1-C2	307.RY(1)C9	0.51	2.00	0.029
17.BD(1)C1-C2	333.RY(1)C10	0.51	2.00	0.029
18.BD(2)C1-C2	66.BD*(2)C3-C5	13.82	0.22	0.050
18.BD(2)C1-C2	69.BD*(2)C4-C6	13.82	0.22	0.050
18.BD(2)C1-C2	76.BD*(2)C7-C9	15.36	0.21	0.051
18.BD(2)C1-C2	79.BD*(2)C8-C10	15.36	0.21	0.051
18.BD(2)C1-C2	309.RY(3)C9	1.09	0.79	0.026
18.BD(2)C1-C2	335.RY(3)C10	1.09	0.79	0.026
19.BD(1)C1-C3	59.BD*(1)C1-C2	0.72	0.94	0.023
19.BD(1)C1-C3	62.BD*(1)C1-C4	0.95	0.95	0.027
19.BD(1)C1-C3	64.BD*(1)C2-C10	2.64	0.95	0.045
19.BD(1)C1-C3	65.BD*(1)C3-C5	0.86	0.99	0.026
19.BD(1)C1-C3	67.BD*(1)C3-B11	1.42	0.90	0.032
19.BD(1)C1-C3	68.BD*(1)C4-C6	2.37	0.99	0.043
19.BD(1)C1-C3	72.BD*(1)C5-H29	2.85	0.86	0.044
19.BD(1)C1-C3	125.RY(1)C2	1.17	1.88	0.042
19.BD(1)C1-C3	177.RY(1)C4	0.53	1.88	0.028
19.BD(1)C1-C3	203.RY(1)C5	0.76	1.87	0.034
20.BD(1)C1-C4	59.BD*(1)C1-C2	0.72	0.94	0.023
20.BD(1)C1-C4	61.BD*(1)C1-C3	0.95	0.95	0.027
20.BD(1)C1-C4	63.BD*(1)C2-C9	2.64	0.95	0.045
20.BD(1)C1-C4	65.BD*(1)C3-C5	2.37	0.99	0.043
20.BD(1)C1-C4	68.BD*(1)C4-C6	0.86	0.99	0.026
20.BD(1)C1-C4	70.BD*(1)C4-B12	1.42	0.90	0.032
20.BD(1)C1-C4	74.BD*(1)C6-H30	2.85	0.86	0.044
20.BD(1)C1-C4	125.RY(1)C2	1.17	1.88	0.042
20.BD(1)C1-C4	151.RY(1)C3	0.53	1.88	0.028
20.BD(1)C1-C4	229.RY(1)C6	0.76	1.87	0.034
21.BD(1)C2-C9	59.BD*(1)C1-C2	0.87	0.96	0.026
21.BD(1)C2-C9	62.BD*(1)C1-C4	2.75	0.97	0.046
21.BD(1)C2-C9	64.BD*(1)C2-C10	0.73	0.97	0.024
21.BD(1)C2-C9	75.BD*(1)C7-C9	0.68	1.02	0.024
21.BD(1)C2-C9	77.BD*(1)C7-H31	2.52	0.87	0.042
21.BD(1)C2-C9	78.BD*(1)C8-C10	1.86	1.02	0.039
21.BD(1)C2-C9	99.RY(1)C1	1.25	1.88	0.043
21.BD(1)C2-C9	255.RY(1)C7	0.68	1.99	0.033
21.BD(1)C2-C9	256.RY(2)C7	0.55	1.63	0.027
21.BD(1)C2-C9	333.RY(1)C10	0.99	2.02	0.040
22.BD(1)C2-C10	59.BD*(1)C1-C2	0.87	0.96	0.026
22.BD(1)C2-C10	61.BD*(1)C1-C3	2.75	0.97	0.046
22.BD(1)C2-C10	63.BD*(1)C2-C9	0.73	0.97	0.024
22.BD(1)C2-C10	75.BD*(1)C7-C9	1.86	1.02	0.039
22.BD(1)C2-C10	78.BD*(1)C8-C10	0.68	1.02	0.024
22.BD(1)C2-C10	80.BD*(1)C8-H32	2.52	0.87	0.042
22.BD(1)C2-C10	99.RY(1)C1	1.25	1.88	0.043
22.BD(1)C2-C10	281.RY(1)C8	0.68	1.99	0.033
22.BD(1)C2-C10	282.RY(2)C8	0.55	1.63	0.027
22.BD(1)C2-C10	307.RY(1)C9	0.99	2.02	0.040

23.BD(1)C3-C5	57.LV(1)B11	1.82	0.51	0.027
23.BD(1)C3-C5	61.BD*(1)C1-C3	1.00	0.97	0.028
23.BD(1)C3-C5	62.BD*(1)C1-C4	3.30	0.97	0.050
23.BD(1)C3-C5	67.BD*(1)C3-B11	1.66	0.91	0.035
23.BD(1)C3-C5	71.BD*(1)C5-C7	0.76	0.98	0.024
23.BD(1)C3-C5	77.BD*(1)C7-H31	2.09	0.87	0.038
23.BD(1)C3-C5	83.BD*(1)B11-C13	0.64	0.88	0.021
23.BD(1)C3-C5	99.RY(1)C1	0.79	1.88	0.034
23.BD(1)C3-C5	100.RY(2)C1	0.80	2.02	0.036
23.BD(1)C3-C5	255.RY(1)C7	0.63	1.99	0.032
24.BD(2)C3-C5	57.LV(1)B11	15.84	0.22	0.052
24.BD(2)C3-C5	60.BD*(2)C1-C2	14.23	0.23	0.051
24.BD(2)C3-C5	76.BD*(2)C7-C9	14.04	0.22	0.050
24.BD(2)C3-C5	83.BD*(1)B11-C13	1.55	0.59	0.027
24.BD(2)C3-C5	84.BD*(1)B11-C17	0.75	0.59	0.019
24.BD(2)C3-C5	101.RY(3)C1	0.94	0.86	0.025
24.BD(2)C3-C5	257.RY(3)C7	0.80	0.97	0.025
25.BD(1)C3-B11	59.BD*(1)C1-C2	3.96	0.83	0.051
25.BD(1)C3-B11	61.BD*(1)C1-C3	0.96	0.84	0.025
25.BD(1)C3-B11	65.BD*(1)C3-C5	0.85	0.88	0.024
25.BD(1)C3-B11	71.BD*(1)C5-C7	4.42	0.86	0.055
25.BD(1)C3-B11	72.BD*(1)C5-H29	0.51	0.75	0.017
25.BD(1)C3-B11	89.BD*(1)C13-H16	1.40	0.73	0.028
25.BD(1)C3-B11	91.BD*(1)C17-H19	1.12	0.72	0.025
25.BD(1)C3-B11	99.RY(1)C1	0.91	1.76	0.036
25.BD(1)C3-B11	100.RY(2)C1	1.81	1.89	0.052
25.BD(1)C3-B11	203.RY(1)C5	1.59	1.76	0.047
26.BD(1)C4-C6	58.LV(1)B12	1.82	0.51	0.027
26.BD(1)C4-C6	61.BD*(1)C1-C3	3.30	0.97	0.050
26.BD(1)C4-C6	62.BD*(1)C1-C4	1.00	0.97	0.028
26.BD(1)C4-C6	70.BD*(1)C4-B12	1.66	0.91	0.035
26.BD(1)C4-C6	73.BD*(1)C6-C8	0.76	0.98	0.024
26.BD(1)C4-C6	80.BD*(1)C8-H32	2.09	0.87	0.038
26.BD(1)C4-C6	85.BD*(1)B12-C21	0.64	0.88	0.021
26.BD(1)C4-C6	99.RY(1)C1	0.79	1.88	0.034
26.BD(1)C4-C6	100.RY(2)C1	0.80	2.02	0.036
26.BD(1)C4-C6	281.RY(1)C8	0.63	1.99	0.032
27.BD(2)C4-C6	58.LV(1)B12	15.83	0.22	0.052
27.BD(2)C4-C6	60.BD*(2)C1-C2	14.23	0.23	0.051
27.BD(2)C4-C6	79.BD*(2)C8-C10	14.04	0.22	0.050
27.BD(2)C4-C6	85.BD*(1)B12-C21	1.55	0.59	0.027
27.BD(2)C4-C6	86.BD*(1)B12-C25	0.75	0.59	0.019
27.BD(2)C4-C6	101.RY(3)C1	0.94	0.86	0.025
27.BD(2)C4-C6	283.RY(3)C8	0.80	0.97	0.025
28.BD(1)C4-B12	59.BD*(1)C1-C2	3.96	0.83	0.051
28.BD(1)C4-B12	62.BD*(1)C1-C4	0.96	0.84	0.025
28.BD(1)C4-B12	68.BD*(1)C4-C6	0.85	0.88	0.024
28.BD(1)C4-B12	73.BD*(1)C6-C8	4.42	0.86	0.055
28.BD(1)C4-B12	74.BD*(1)C6-H30	0.51	0.75	0.017
28.BD(1)C4-B12	95.BD*(1)C21-H24	1.40	0.73	0.028
28.BD(1)C4-B12	97.BD*(1)C25-H27	1.12	0.72	0.025
28.BD(1)C4-B12	99.RY(1)C1	0.92	1.76	0.036
28.BD(1)C4-B12	100.RY(2)C1	1.81	1.89	0.052
28.BD(1)C4-B12	229.RY(1)C6	1.59	1.76	0.047
29.BD(1)C5-C7	65.BD*(1)C3-C5	0.86	1.01	0.026
29.BD(1)C5-C7	67.BD*(1)C3-B11	2.30	0.92	0.041
29.BD(1)C5-C7	75.BD*(1)C7-C9	0.79	1.03	0.025
29.BD(1)C5-C7	81.BD*(1)C9-H33	2.59	0.87	0.042
29.BD(1)C5-C7	151.RY(1)C3	1.54	1.90	0.048

29.BD(1)C5-C7	307.RY(1)C9	0.74	2.02	0.034
30.BD(1)C5-H29	57.LV(1)B11	0.66	0.41	0.015
30.BD(1)C5-H29	61.BD*(1)C1-C3	4.87	0.87	0.058
30.BD(1)C5-H29	75.BD*(1)C7-C9	3.52	0.93	0.051
30.BD(1)C5-H29	77.BD*(1)C7-H31	0.62	0.77	0.020
30.BD(1)C5-H29	151.RY(1)C3	1.49	1.80	0.046
30.BD(1)C5-H29	255.RY(1)C7	1.13	1.89	0.041
31.BD(1)C6-C8	68.BD*(1)C4-C6	0.86	1.01	0.026
31.BD(1)C6-C8	70.BD*(1)C4-B12	2.30	0.92	0.041
31.BD(1)C6-C8	78.BD*(1)C8-C10	0.79	1.03	0.025
31.BD(1)C6-C8	82.BD*(1)C10-H34	2.59	0.87	0.042
31.BD(1)C6-C8	177.RY(1)C4	1.54	1.90	0.048
31.BD(1)C6-C8	333.RY(1)C10	0.74	2.02	0.034
32.BD(1)C6-H30	58.LV(1)B12	0.66	0.41	0.015
32.BD(1)C6-H30	62.BD*(1)C1-C4	4.87	0.87	0.058
32.BD(1)C6-H30	78.BD*(1)C8-C10	3.52	0.93	0.051
32.BD(1)C6-H30	80.BD*(1)C8-H32	0.62	0.77	0.020
32.BD(1)C6-H30	177.RY(1)C4	1.49	1.80	0.046
32.BD(1)C6-H30	281.RY(1)C8	1.13	1.89	0.041
33.BD(1)C7-C9	63.BD*(1)C2-C9	0.78	0.99	0.025
33.BD(1)C7-C9	64.BD*(1)C2-C10	2.65	0.99	0.046
33.BD(1)C7-C9	71.BD*(1)C5-C7	0.87	1.00	0.026
33.BD(1)C7-C9	72.BD*(1)C5-H29	2.02	0.89	0.038
33.BD(1)C7-C9	125.RY(1)C2	0.68	1.92	0.032
33.BD(1)C7-C9	126.RY(2)C2	0.94	2.11	0.040
33.BD(1)C7-C9	203.RY(1)C5	0.95	1.91	0.038
34.BD(2)C7-C9	60.BD*(2)C1-C2	13.40	0.24	0.050
34.BD(2)C7-C9	66.BD*(2)C3-C5	13.72	0.24	0.051
34.BD(2)C7-C9	204.RY(2)C5	0.88	0.79	0.024
35.BD(1)C7-H31	63.BD*(1)C2-C9	4.09	0.88	0.053
35.BD(1)C7-H31	65.BD*(1)C3-C5	4.04	0.91	0.054
35.BD(1)C7-H31	72.BD*(1)C5-H29	0.57	0.78	0.019
35.BD(1)C7-H31	81.BD*(1)C9-H33	0.60	0.77	0.019
35.BD(1)C7-H31	203.RY(1)C5	1.03	1.80	0.038
35.BD(1)C7-H31	307.RY(1)C9	1.29	1.92	0.045
36.BD(1)C8-C10	63.BD*(1)C2-C9	2.65	0.99	0.046
36.BD(1)C8-C10	64.BD*(1)C2-C10	0.78	0.99	0.025
36.BD(1)C8-C10	73.BD*(1)C6-C8	0.87	1.00	0.026
36.BD(1)C8-C10	74.BD*(1)C6-H30	2.02	0.89	0.038
36.BD(1)C8-C10	125.RY(1)C2	0.68	1.92	0.032
36.BD(1)C8-C10	126.RY(2)C2	0.94	2.11	0.040
36.BD(1)C8-C10	229.RY(1)C6	0.95	1.91	0.038
37.BD(2)C8-C10	60.BD*(2)C1-C2	13.40	0.24	0.050
37.BD(2)C8-C10	69.BD*(2)C4-C6	13.72	0.24	0.051
37.BD(2)C8-C10	230.RY(2)C6	0.88	0.79	0.024
38.BD(1)C8-H32	64.BD*(1)C2-C10	4.09	0.88	0.053
38.BD(1)C8-H32	68.BD*(1)C4-C6	4.04	0.91	0.054
38.BD(1)C8-H32	74.BD*(1)C6-H30	0.57	0.78	0.019
38.BD(1)C8-H32	82.BD*(1)C10-H34	0.60	0.77	0.019
38.BD(1)C8-H32	229.RY(1)C6	1.03	1.80	0.038
38.BD(1)C8-H32	333.RY(1)C10	1.29	1.92	0.045
39.BD(1)C9-H33	59.BD*(1)C1-C2	4.80	0.87	0.058
39.BD(1)C9-H33	71.BD*(1)C5-C7	3.92	0.90	0.053
39.BD(1)C9-H33	77.BD*(1)C7-H31	0.64	0.78	0.020
39.BD(1)C9-H33	125.RY(1)C2	0.52	1.81	0.027
39.BD(1)C9-H33	126.RY(2)C2	1.14	2.00	0.043
39.BD(1)C9-H33	255.RY(1)C7	1.22	1.90	0.043
40.BD(1)C10-H34	59.BD*(1)C1-C2	4.80	0.87	0.058
40.BD(1)C10-H34	73.BD*(1)C6-C8	3.92	0.90	0.053

40.BD(1)C10-H34	80.BD*(1)C8-H32	0.64	0.78	0.020
40.BD(1)C10-H34	125.RY(1)C2	0.52	1.81	0.027
40.BD(1)C10-H34	126.RY(2)C2	1.14	2.00	0.043
40.BD(1)C10-H34	281.RY(1)C8	1.22	1.90	0.043
41.BD(1)B11-C13	58.LV(1)B12	1.62	0.39	0.022
41.BD(1)B11-C13	65.BD*(1)C3-C5	1.65	0.88	0.034
41.BD(1)B11-C13	66.BD*(2)C3-C5	1.71	0.40	0.023
41.BD(1)B11-C13	87.BD*(1)C13-H14	0.80	0.72	0.021
41.BD(1)B11-C13	88.BD*(1)C13-H15	0.81	0.75	0.022
41.BD(1)B11-C13	89.BD*(1)C13-H16	0.81	0.73	0.022
41.BD(1)B11-C13	92.BD*(1)C17-H20	2.06	0.74	0.035
41.BD(1)B11-C13	152.RY(2)C3	0.56	1.12	0.022
41.BD(1)B11-C13	437.RY(1)H14	0.52	2.04	0.029
42.BD(1)B11-C17	61.BD*(1)C1-C3	2.77	0.84	0.043
42.BD(1)B11-C17	66.BD*(2)C3-C5	0.74	0.40	0.015
42.BD(1)B11-C17	88.BD*(1)C13-H15	2.10	0.75	0.036
42.BD(1)B11-C17	90.BD*(1)C17-H18	0.92	0.72	0.023
42.BD(1)B11-C17	91.BD*(1)C17-H19	0.82	0.73	0.022
42.BD(1)B11-C17	92.BD*(1)C17-H20	0.79	0.74	0.022
43.BD(1)B12-C21	57.LV(1)B11	1.62	0.39	0.022
43.BD(1)B12-C21	68.BD*(1)C4-C6	1.65	0.88	0.034
43.BD(1)B12-C21	69.BD*(2)C4-C6	1.71	0.40	0.023
43.BD(1)B12-C21	93.BD*(1)C21-H22	0.80	0.72	0.021
43.BD(1)B12-C21	94.BD*(1)C21-H23	0.81	0.75	0.022
43.BD(1)B12-C21	95.BD*(1)C21-H24	0.81	0.73	0.022
43.BD(1)B12-C21	98.BD*(1)C25-H28	2.06	0.74	0.035
43.BD(1)B12-C21	178.RY(2)C4	0.56	1.12	0.022
43.BD(1)B12-C21	567.RY(1)H22	0.52	2.04	0.029
44.BD(1)B12-C25	62.BD*(1)C1-C4	2.77	0.84	0.043
44.BD(1)B12-C25	69.BD*(2)C4-C6	0.74	0.40	0.015
44.BD(1)B12-C25	94.BD*(1)C21-H23	2.10	0.75	0.036
44.BD(1)B12-C25	96.BD*(1)C25-H26	0.92	0.72	0.023
44.BD(1)B12-C25	97.BD*(1)C25-H27	0.82	0.73	0.022
44.BD(1)B12-C25	98.BD*(1)C25-H28	0.79	0.74	0.022
45.BD(1)C13-H14	57.LV(1)B11	11.31	0.39	0.059
45.BD(1)C13-H14	67.BD*(1)C3-B11	0.54	0.79	0.018
45.BD(1)C13-H14	83.BD*(1)B11-C13	0.85	0.76	0.023
46.BD(1)C13-H15	58.LV(1)B12	2.19	0.39	0.026
46.BD(1)C13-H15	84.BD*(1)B11-C17	2.47	0.77	0.039
46.BD(1)C13-H15	360.RY(2)B11	0.51	1.14	0.022
47.BD(1)C13-H16	57.LV(1)B11	2.39	0.39	0.027
47.BD(1)C13-H16	58.LV(1)B12	0.58	0.39	0.013
47.BD(1)C13-H16	67.BD*(1)C3-B11	2.06	0.79	0.036
47.BD(1)C13-H16	359.RY(1)B11	0.67	1.25	0.026
48.BD(1)C17-H18	57.LV(1)B11	8.87	0.39	0.052
48.BD(1)C17-H18	67.BD*(1)C3-B11	0.78	0.79	0.022
48.BD(1)C17-H18	84.BD*(1)B11-C17	0.64	0.76	0.020
49.BD(1)C17-H19	57.LV(1)B11	3.89	0.39	0.035
49.BD(1)C17-H19	67.BD*(1)C3-B11	1.87	0.79	0.034
49.BD(1)C17-H19	84.BD*(1)B11-C17	0.53	0.76	0.018
49.BD(1)C17-H19	359.RY(1)B11	0.65	1.24	0.025
50.BD(1)C17-H20	83.BD*(1)B11-C13	2.72	0.76	0.041
50.BD(1)C17-H20	84.BD*(1)B11-C17	0.54	0.76	0.018
50.BD(1)C17-H20	360.RY(2)B11	0.65	1.13	0.024
50.BD(1)C17-H20	361.RY(3)B11	0.60	2.17	0.032
51.BD(1)C21-H22	58.LV(1)B12	11.31	0.39	0.059
51.BD(1)C21-H22	70.BD*(1)C4-B12	0.54	0.79	0.018
51.BD(1)C21-H22	85.BD*(1)B12-C21	0.85	0.76	0.023
52.BD(1)C21-H23	57.LV(1)B11	2.18	0.39	0.026

52.BD(1)C21-H23	86.BD*(1)B12-C25	2.47	0.77	0.039
52.BD(1)C21-H23	386.RY(2)B12	0.51	1.14	0.022
53.BD(1)C21-H24	57.LV(1)B11	0.58	0.39	0.013
53.BD(1)C21-H24	58.LV(1)B12	2.39	0.39	0.027
53.BD(1)C21-H24	70.BD*(1)C4-B12	2.06	0.79	0.036
53.BD(1)C21-H24	385.RY(1)B12	0.67	1.25	0.026
54.BD(1)C25-H26	58.LV(1)B12	8.87	0.39	0.052
54.BD(1)C25-H26	70.BD*(1)C4-B12	0.78	0.79	0.022
54.BD(1)C25-H26	86.BD*(1)B12-C25	0.64	0.76	0.020
55.BD(1)C25-H27	58.LV(1)B12	3.90	0.39	0.035
55.BD(1)C25-H27	70.BD*(1)C4-B12	1.87	0.79	0.034
55.BD(1)C25-H27	86.BD*(1)B12-C25	0.53	0.76	0.018
55.BD(1)C25-H27	385.RY(1)B12	0.65	1.24	0.025
56.BD(1)C25-H28	85.BD*(1)B12-C21	2.72	0.76	0.041
56.BD(1)C25-H28	86.BD*(1)B12-C25	0.54	0.76	0.018
56.BD(1)C25-H28	386.RY(2)B12	0.65	1.13	0.024
56.BD(1)C25-H28	387.RY(3)B12	0.60	2.17	0.032

Table S20. Natural Bond Orbitals Summary for **1**, without Rydberg orbitals.

NBO	Occupancy	Energy / a.u.	Principal delocalizations (geminal,vicinal,remote)
1.CR(1)C1	1.99998	-9.89874	
2.CR(1)C2	1.99998	-9.89858	
3.CR(1)C3	1.99998	-9.87444	
4.CR(1)C4	1.99998	-9.87444	
5.CR(1)C5	1.99998	-9.89187	
6.CR(1)C6	1.99998	-9.89187	
7.CR(1)C7	1.99998	-9.88954	
8.CR(1)C8	1.99998	-9.88954	
9.CR(1)C9	1.99998	-9.89305	
10.CR(1)C10	1.99998	-9.89305	
11.CR(1)B11	1.99996	-6.49117	
12.CR(1)B12	1.99996	-6.49117	
13.CR(1)C13	1.99998	-9.85404	
14.CR(1)C17	1.99998	-9.85152	
15.CR(1)C21	1.99998	-9.85404	
16.CR(1)C25	1.99998	-9.85152	
17.BD(1)C1-C2	1.97015	-0.50563	67(v),70(v),81(v),82(v)
			151(v),177(v),63(g),64(g)
			61(g),62(g),307(v),333(v)
18.BD(2)C1-C2	1.51985	-0.21742	76(v),79(v),69(v),66(v)
			309(v),335(v)
19.BD(1)C1-C3	1.96917	-0.50069	72(v),64(v),68(v),67(g)
			125(v),62(g),65(g),203(v)
			59(g),177(v)
20.BD(1)C1-C4	1.96917	-0.50069	74(v),63(v),65(v),70(g)
			125(v),61(g),68(g),229(v)
			59(g),151(v)
21.BD(1)C2-C9	1.97722	-0.51919	62(v),77(v),78(v),99(v)
			333(v),59(g),64(g),75(g)
			255(v),256(v)
22.BD(1)C2-C10	1.97722	-0.51919	61(v),80(v),75(v),99(v)
			307(v),59(g),63(g),78(g)
			281(v),282(v)
23.BD(1)C3-C5	1.97085	-0.51833	62(v),77(v),57(v),67(g)
			61(g),100(v),99(v),71(g)
			83(v),255(v)
24.BD(2)C3-C5	1.67412	-0.22428	57(v),60(v),76(v),83(v)
			101(v),257(v),84(v)
25.BD(1)C3-B11	1.95416	-0.39002	71(v),59(v),100(v),203(v)
			89(v),91(v),61(g),99(v)
			65(g),72(v)
26.BD(1)C4-C6	1.97085	-0.51833	61(v),80(v),58(v),70(g)
			62(g),100(v),99(v),73(g)
			85(v),281(v)

27.BD(2)C4-C6	1.67412	-0.22428	58(v),60(v),79(v),85(v)
			101(v),283(v),86(v)
28.BD(1)C4-B12	1.95416	-0.39002	73(v),59(v),100(v),229(v)
			95(v),97(v),62(g),99(v)
			68(g),74(v)
29.BD(1)C5-C7	1.98223	-0.52409	81(v),67(v),151(v),65(g)
			75(g),307(v)
30.BD(1)C5-H29	1.97255	-0.42171	61(v),75(v),151(v),255(v)
			57(r),77(v)
31.BD(1)C6-C8	1.98223	-0.52409	82(v),70(v),177(v),68(g)
			78(g),333(v)
32.BD(1)C6-H30	1.97255	-0.42171	62(v),78(v),177(v),281(v)
			58(r),80(v)
33.BD(1)C7-C9	1.98394	-0.53805	64(v),72(v),203(v),126(v)
			71(g),63(g),125(v)
34.BD(2)C7-C9	1.72001	-0.23462	66(v),60(v),204(v)
35.BD(1)C7-H31	1.97731	-0.42704	63(v),65(v),307(v),203(v)
			81(v),72(v)
36.BD(1)C8-C10	1.98394	-0.53805	63(v),74(v),229(v),126(v)
			73(g),64(g),125(v)
37.BD(2)C8-C10	1.72001	-0.23462	69(v),60(v),230(v)
38.BD(1)C8-H32	1.97731	-0.42704	64(v),68(v),333(v),229(v)
			82(v),74(v)
39.BD(1)C9-H33	1.97679	-0.42881	59(v),71(v),255(v),126(v)
			77(v),125(v)
40.BD(1)C10-H34	1.97679	-0.42881	59(v),73(v),281(v),126(v)
			80(v),125(v)
41.BD(1)B11-C13	1.96549	-0.39478	92(v),66(v),65(v),58(r)
			88(g),89(g),87(g),152(v)
			437(v)
42.BD(1)B11-C17	1.97432	-0.39482	61(v),88(v),90(g),91(g)
			92(g),66(v)
43.BD(1)B12-C21	1.96549	-0.39478	98(v),69(v),68(v),57(r)
			94(g),95(g),93(g),178(v)
			567(v)
44.BD(1)B12-C25	1.97432	-0.39482	62(v),94(v),96(g),97(g)
			98(g),69(v)
45.BD(1)C13-H14	1.94009	-0.39605	57(v),83(g),67(v)
46.BD(1)C13-H15	1.97627	-0.39974	84(v),58(r),360(v)
47.BD(1)C13-H16	1.97306	-0.39986	57(v),67(v),359(v),58(r)
48.BD(1)C17-H18	1.95296	-0.39602	57(v),67(v),84(g)
49.BD(1)C17-H19	1.96867	-0.39710	57(v),67(v),359(v),84(g)
50.BD(1)C17-H20	1.98379	-0.39817	83(v),360(v),361(v),84(g)
51.BD(1)C21-H22	1.94009	-0.39605	58(v),85(g),70(v)
52.BD(1)C21-H23	1.97628	-0.39974	86(v),57(r),386(v)
53.BD(1)C21-H24	1.97307	-0.39986	58(v),70(v),385(v),57(r)
54.BD(1)C25-H26	1.95298	-0.39602	58(v),70(v),86(g)
55.BD(1)C25-H27	1.96865	-0.39710	58(v),70(v),385(v),86(g)
56.BD(1)C25-H28	1.98379	-0.39817	85(v),386(v),387(v),86(g)
Non-Lewis			
57.LV(1)B11	0.23150	-0.00823	
58.LV(1)B12	0.23149	-0.00823	
59.BD*(1)C1-C2	0.03793	0.43880	
60.BD*(2)C1-C2	0.44639	0.00398	
61.BD*(1)C1-C3	0.03161	0.44884	
62.BD*(1)C1-C4	0.03161	0.44885	
63.BD*(1)C2-C9	0.02050	0.44960	
64.BD*(1)C2-C10	0.02050	0.44960	
65.BD*(1)C3-C5	0.02109	0.48645	
66.BD*(2)C3-C5	0.28207	0.00660	
67.BD*(1)C3-B11	0.02793	0.39462	
68.BD*(1)C4-C6	0.02109	0.48645	
69.BD*(2)C4-C6	0.28207	0.00660	
70.BD*(1)C4-B12	0.02794	0.39462	
71.BD*(1)C5-C7	0.01873	0.46630	
72.BD*(1)C5-H29	0.01765	0.35570	
73.BD*(1)C6-C8	0.01873	0.46630	
74.BD*(1)C6-H30	0.01765	0.35570	
75.BD*(1)C7-C9	0.01242	0.50516	
76.BD*(2)C7-C9	0.26030	-0.00283	
77.BD*(1)C7-H31	0.01584	0.34824	
78.BD*(1)C8-C10	0.01242	0.50516	
79.BD*(2)C8-C10	0.26031	-0.00283	

80.BD*(1)C8-H32	0.01584	0.34824	
81.BD*(1)C9-H33	0.01626	0.34635	
82.BD*(1)C10-H34	0.01626	0.34635	
83.BD*(1)B11-C13	0.01749	0.36417	
84.BD*(1)B11-C17	0.01466	0.36646	
85.BD*(1)B12-C21	0.01749	0.36416	
86.BD*(1)B12-C25	0.01466	0.36646	
87.BD*(1)C13-H14	0.00573	0.32585	
88.BD*(1)C13-H15	0.00944	0.35730	
89.BD*(1)C13-H16	0.00861	0.33620	
90.BD*(1)C17-H18	0.00517	0.32748	
91.BD*(1)C17-H19	0.00832	0.33309	
92.BD*(1)C17-H20	0.00981	0.34455	
93.BD*(1)C21-H22	0.00573	0.32585	
94.BD*(1)C21-H23	0.00944	0.35730	
95.BD*(1)C21-H24	0.00861	0.33620	
96.BD*(1)C25-H26	0.00517	0.32749	
97.BD*(1)C25-H27	0.00831	0.33307	
98.BD*(1)C25-H28	0.00981	0.34455	

Table S21. Second order perturbation analysis of the Fock matrix. In NBO-basis for [**1**-OH]$^-$. Threshold for printing the donor acceptor interactions in 0.50 kcal/mol. E(2) is the energy of the donor-acceptor interaction in kcal/mol, E(NL) – E(L) is the energy difference between the donor and acceptor in atomic units and F(L,NL) is the overlap between the donor and acceptor natural orbitals in atomic units.

Donor (L) NBO	Acceptor (NL) NBO	E(2) / kcal/mol	E(NL) – E(L) / a.u	F(L,NL) / a.u.
18.LP(1)C5	62.LV(1)C4	1211.00	0.01	0.108
18.LP(1)C5	65.BD*(2)C1-C6	80.70	0.12	0.087
18.LP(1)C5	68.BD*(2)C2-C3	1.75	0.09	0.011
18.LP(1)C5	78.BD*(2)C7-C8	80.70	0.12	0.087
18.LP(1)C5	83.BD*(2)C9-C10	1.75	0.09	0.011
18.LP(1)C5	185.RY(3)C4	1.75	0.59	0.029
18.LP(1)C5	190.RY(8)C4	1.07	2.80	0.049
18.LP(1)C5	211.RY(3)C5	3.80	0.69	0.046
18.LP(1)C5	236.RY(2)C6	0.98	0.72	0.024
18.LP(1)C5	240.RY(6)C6	0.85	2.44	0.041
18.LP(1)C5	262.RY(2)C7	0.98	0.72	0.024
18.LP(1)C5	266.RY(6)C7	0.84	2.44	0.041
19.LP(1)O35	76.BD*(1)C6-B14	3.11	0.70	0.042
19.LP(1)O35	79.BD*(1)C7-B15	3.11	0.70	0.042
19.LP(1)O35	87.BD*(1)B14-C22	2.25	0.67	0.035
19.LP(1)O35	89.BD*(1)B15-C19	2.25	0.67	0.035
19.LP(1)O35	781.RY(1)H36	1.33	2.11	0.047
20.BD(1)C1-C2	64.BD*(1)C1-C6	0.97	1.03	0.028
20.BD(1)C1-C2	67.BD*(1)C2-C3	0.89	1.02	0.027
20.BD(1)C1-C2	71.BD*(1)C3-H13	2.79	0.85	0.044
20.BD(1)C1-C2	76.BD*(1)C6-B14	1.96	0.90	0.038
20.BD(1)C1-C2	157.RY(1)C3	0.73	1.99	0.034
20.BD(1)C1-C2	235.RY(1)C6	1.55	2.10	0.051
21.BD(1)C1-C6	63.BD*(1)C1-C2	0.98	0.98	0.028
21.BD(1)C1-C6	69.BD*(1)C2-H12	2.27	0.84	0.039
21.BD(1)C1-C6	74.BD*(1)C5-C6	0.73	0.97	0.024
21.BD(1)C1-C6	75.BD*(1)C5-C7	3.43	0.97	0.051
21.BD(1)C1-C6	76.BD*(1)C6-B14	1.30	0.89	0.030
21.BD(1)C1-C6	88.BD*(1)B14-O35	0.77	0.76	0.022
21.BD(1)C1-C6	131.RY(1)C2	0.62	1.92	0.031
21.BD(1)C1-C6	133.RY(3)C2	0.53	1.78	0.027
21.BD(1)C1-C6	209.RY(1)C5	1.30	1.99	0.045
21.BD(1)C1-C6	210.RY(2)C5	0.65	2.14	0.033
21.BD(1)C1-C6	407.RY(4)B14	0.71	2.23	0.035
22.BD(2)C1-C6	68.BD*(2)C2-C3	17.69	0.21	0.054
22.BD(2)C1-C6	86.BD*(1)B14-C21	1.38	0.56	0.025
22.BD(2)C1-C6	87.BD*(1)B14-C22	2.39	0.56	0.033
22.BD(2)C1-C6	132.RY(2)C2	1.58	0.72	0.030
22.BD(2)C1-C6	211.RY(3)C5	0.80	0.81	0.023
23.BD(1)C1-H11	67.BD*(1)C2-C3	3.75	0.92	0.052
23.BD(1)C1-H11	69.BD*(1)C2-H12	0.61	0.75	0.019
23.BD(1)C1-H11	74.BD*(1)C5-C6	5.29	0.88	0.061
23.BD(1)C1-H11	131.RY(1)C2	1.08	1.82	0.040
23.BD(1)C1-H11	235.RY(1)C6	1.99	2.00	0.056
23.BD(1)C1-H11	241.RY(7)C6	0.53	3.58	0.039
24.BD(1)C2-C3	63.BD*(1)C1-C2	0.95	1.01	0.028
24.BD(1)C2-C3	66.BD*(1)C1-H11	2.08	0.89	0.038
24.BD(1)C2-C3	70.BD*(1)C3-C4	0.92	0.99	0.027
24.BD(1)C2-C3	73.BD*(1)C4-C10	2.66	0.99	0.046
24.BD(1)C2-C3	105.RY(1)C1	0.99	1.94	0.039
24.BD(1)C2-C3	183.RY(1)C4	0.69	1.88	0.032
24.BD(1)C2-C3	184.RY(2)C4	0.81	2.12	0.037
25.BD(2)C2-C3	62.LV(1)C4	50.83	0.13	0.072
25.BD(2)C2-C3	65.BD*(2)C1-C6	10.94	0.26	0.048
25.BD(2)C2-C3	106.RY(2)C1	1.22	0.73	0.027
25.BD(2)C2-C3	185.RY(3)C4	0.69	0.73	0.020
26.BD(1)C2-H12	64.BD*(1)C1-C6	3.97	0.95	0.055
26.BD(1)C2-H12	66.BD*(1)C1-H11	0.55	0.79	0.019
26.BD(1)C2-H12	70.BD*(1)C3-C4	4.05	0.89	0.054
26.BD(1)C2-H12	71.BD*(1)C3-H13	0.57	0.77	0.019
26.BD(1)C2-H12	105.RY(1)C1	1.18	1.84	0.042
26.BD(1)C2-H12	157.RY(1)C3	1.30	1.91	0.044
27.BD(1)C3-C4	67.BD*(1)C2-C3	0.84	1.02	0.026
27.BD(1)C3-C4	69.BD*(1)C2-H12	2.74	0.85	0.043

27.BD(1)C3-C4	72.BD*(1)C4-C5	0.84	0.95	0.025
27.BD(1)C3-C4	73.BD*(1)C4-C10	0.74	0.97	0.024
27.BD(1)C3-C4	75.BD*(1)C5-C7	2.60	0.98	0.045
27.BD(1)C3-C4	82.BD*(1)C9-C10	1.93	1.02	0.040
27.BD(1)C3-C4	131.RY(1)C2	0.68	1.92	0.032
27.BD(1)C3-C4	133.RY(3)C2	0.57	1.79	0.029
27.BD(1)C3-C4	209.RY(1)C5	1.29	1.99	0.045
27.BD(1)C3-C4	339.RY(1)C10	0.97	1.99	0.039
28.BD(1)C3-H13	63.BD*(1)C1-C2	3.85	0.90	0.053
28.BD(1)C3-H13	69.BD*(1)C2-H12	0.57	0.77	0.019
28.BD(1)C3-H13	72.BD*(1)C4-C5	4.63	0.87	0.057
28.BD(1)C3-H13	131.RY(1)C2	1.21	1.84	0.042
28.BD(1)C3-H13	183.RY(1)C4	0.55	1.78	0.028
28.BD(1)C3-H13	184.RY(2)C4	1.10	2.01	0.042
29.BD(1)C4-C5	70.BD*(1)C3-C4	0.67	0.95	0.023
29.BD(1)C4-C5	71.BD*(1)C3-H13	2.45	0.83	0.040
29.BD(1)C4-C5	73.BD*(1)C4-C10	0.67	0.95	0.023
29.BD(1)C4-C5	74.BD*(1)C5-C6	0.67	0.96	0.023
29.BD(1)C4-C5	75.BD*(1)C5-C7	0.67	0.96	0.023
29.BD(1)C4-C5	76.BD*(1)C6-B14	2.13	0.87	0.039
29.BD(1)C4-C5	79.BD*(1)C7-B15	2.13	0.87	0.039
29.BD(1)C4-C5	85.BD*(1)C10-H18	2.45	0.83	0.040
29.BD(1)C4-C5	159.RY(3)C3	0.54	1.95	0.029
29.BD(1)C4-C5	235.RY(1)C6	0.72	2.07	0.034
29.BD(1)C4-C5	238.RY(4)C6	0.52	3.18	0.036
29.BD(1)C4-C5	261.RY(1)C7	0.72	2.07	0.034
29.BD(1)C4-C5	264.RY(4)C7	0.52	3.18	0.036
29.BD(1)C4-C5	341.RY(3)C10	0.54	1.95	0.029
30.BD(1)C4-C10	67.BD*(1)C2-C3	1.94	1.02	0.040
30.BD(1)C4-C10	70.BD*(1)C3-C4	0.74	0.97	0.024
30.BD(1)C4-C10	72.BD*(1)C4-C5	0.84	0.95	0.025
30.BD(1)C4-C10	74.BD*(1)C5-C6	2.60	0.98	0.045
30.BD(1)C4-C10	82.BD*(1)C9-C10	0.84	1.02	0.026
30.BD(1)C4-C10	84.BD*(1)C9-H17	2.74	0.85	0.043
30.BD(1)C4-C10	157.RY(1)C3	0.97	1.99	0.039
30.BD(1)C4-C10	209.RY(1)C5	1.29	1.99	0.045
30.BD(1)C4-C10	313.RY(1)C9	0.68	1.92	0.032
30.BD(1)C4-C10	315.RY(3)C9	0.57	1.79	0.029
31.BD(1)C5-C6	64.BD*(1)C1-C6	0.56	1.00	0.021
31.BD(1)C5-C6	66.BD*(1)C1-H11	3.24	0.84	0.047
31.BD(1)C5-C6	72.BD*(1)C4-C5	0.66	0.92	0.022
31.BD(1)C5-C6	73.BD*(1)C4-C10	2.65	0.94	0.045
31.BD(1)C5-C6	75.BD*(1)C5-C7	1.02	0.95	0.028
31.BD(1)C5-C6	76.BD*(1)C6-B14	0.79	0.87	0.023
31.BD(1)C5-C6	77.BD*(1)C7-C8	2.53	1.00	0.045
31.BD(1)C5-C6	105.RY(1)C1	0.74	1.89	0.033
31.BD(1)C5-C6	183.RY(1)C4	1.16	1.83	0.041
31.BD(1)C5-C6	261.RY(1)C7	0.72	2.07	0.034
32.BD(1)C5-C7	64.BD*(1)C1-C6	2.53	1.00	0.045
32.BD(1)C5-C7	70.BD*(1)C3-C4	2.65	0.94	0.045
32.BD(1)C5-C7	72.BD*(1)C4-C5	0.66	0.92	0.022
32.BD(1)C5-C7	74.BD*(1)C5-C6	1.02	0.95	0.028
32.BD(1)C5-C7	77.BD*(1)C7-C8	0.56	1.00	0.021
32.BD(1)C5-C7	79.BD*(1)C7-B15	0.78	0.87	0.023
32.BD(1)C5-C7	81.BD*(1)C8-H16	3.24	0.84	0.047
32.BD(1)C5-C7	183.RY(1)C4	1.16	1.83	0.041
32.BD(1)C5-C7	235.RY(1)C6	0.72	2.07	0.034
32.BD(1)C5-C7	287.RY(1)C8	0.74	1.89	0.033
33.BD(1)C6-B14	63.BD*(1)C1-C2	4.64	0.82	0.055
33.BD(1)C6-B14	64.BD*(1)C1-C6	0.64	0.86	0.021
33.BD(1)C6-B14	66.BD*(1)C1-H11	0.73	0.70	0.020
33.BD(1)C6-B14	72.BD*(1)C4-C5	4.19	0.78	0.051
33.BD(1)C6-B14	99.BD*(1)C21-H24	1.51	0.68	0.029
33.BD(1)C6-B14	103.BD*(1)C22-H34	1.61	0.70	0.030
33.BD(1)C6-B14	105.RY(1)C1	2.01	1.75	0.053
33.BD(1)C6-B14	209.RY(1)C5	1.56	1.82	0.048
33.BD(1)C6-B14	210.RY(2)C5	1.77	1.98	0.053
33.BD(1)C6-B14	235.RY(1)C6	0.50	1.93	0.028
33.BD(1)C6-B14	264.RY(4)C7	0.51	3.03	0.035
33.BD(1)C6-B14	425.RY(22)B14	0.51	5.98	0.049
34.BD(1)C7-C8	74.BD*(1)C5-C6	3.43	0.97	0.051
34.BD(1)C7-C8	75.BD*(1)C5-C7	0.73	0.97	0.024
34.BD(1)C7-C8	79.BD*(1)C7-B15	1.30	0.89	0.030

34.BD(1)C7-C8	80.BD*(1)C8-C9	0.98	0.98	0.028
34.BD(1)C7-C8	84.BD*(1)C9-H17	2.27	0.84	0.039
34.BD(1)C7-C8	91.BD*(1)B15-O35	0.77	0.76	0.022
34.BD(1)C7-C8	209.RY(1)C5	1.30	1.99	0.045
34.BD(1)C7-C8	210.RY(2)C5	0.64	2.14	0.033
34.BD(1)C7-C8	313.RY(1)C9	0.62	1.92	0.031
34.BD(1)C7-C8	315.RY(3)C9	0.53	1.78	0.027
34.BD(1)C7-C8	433.RY(4)B15	0.71	2.23	0.035
35.BD(2)C7-C8	83.BD*(2)C9-C10	17.69	0.21	0.054
35.BD(2)C7-C8	89.BD*(1)B15-C19	2.39	0.56	0.033
35.BD(2)C7-C8	90.BD*(1)B15-C20	1.38	0.56	0.025
35.BD(2)C7-C8	211.RY(3)C5	0.80	0.81	0.023
35.BD(2)C7-C8	314.RY(2)C9	1.58	0.72	0.030
36.BD(1)C7-B15	72.BD*(1)C4-C5	4.19	0.78	0.051
36.BD(1)C7-B15	77.BD*(1)C7-C8	0.64	0.86	0.021
36.BD(1)C7-B15	80.BD*(1)C8-C9	4.64	0.82	0.055
36.BD(1)C7-B15	81.BD*(1)C8-H16	0.73	0.70	0.020
36.BD(1)C7-B15	93.BD*(1)C19-H27	1.61	0.70	0.030
36.BD(1)C7-B15	97.BD*(1)C20-H31	1.51	0.68	0.029
36.BD(1)C7-B15	209.RY(1)C5	1.56	1.82	0.048
36.BD(1)C7-B15	210.RY(2)C5	1.77	1.98	0.053
36.BD(1)C7-B15	238.RY(4)C6	0.51	3.03	0.035
36.BD(1)C7-B15	287.RY(1)C8	2.01	1.75	0.053
36.BD(1)C7-B15	451.RY(22)B15	0.51	5.98	0.049
37.BD(1)C8-C9	77.BD*(1)C7-C8	0.97	1.03	0.028
37.BD(1)C8-C9	79.BD*(1)C7-B15	1.96	0.90	0.038
37.BD(1)C8-C9	82.BD*(1)C9-C10	0.89	1.02	0.027
37.BD(1)C8-C9	85.BD*(1)C10-H18	2.79	0.85	0.044
37.BD(1)C8-C9	261.RY(1)C7	1.55	2.10	0.051
37.BD(1)C8-C9	339.RY(1)C10	0.73	1.99	0.034
38.BD(1)C8-H16	75.BD*(1)C5-C7	5.29	0.88	0.061
38.BD(1)C8-H16	82.BD*(1)C9-C10	3.75	0.92	0.052
38.BD(1)C8-H16	84.BD*(1)C9-H17	0.61	0.75	0.019
38.BD(1)C8-H16	261.RY(1)C7	1.99	2.00	0.056
38.BD(1)C8-H16	267.RY(7)C7	0.53	3.58	0.039
38.BD(1)C8-H16	313.RY(1)C9	1.08	1.82	0.040
39.BD(1)C9-C10	70.BD*(1)C3-C4	2.66	0.99	0.046
39.BD(1)C9-C10	73.BD*(1)C4-C10	0.92	0.99	0.027
39.BD(1)C9-C10	80.BD*(1)C8-C9	0.95	1.01	0.028
39.BD(1)C9-C10	81.BD*(1)C8-H16	2.08	0.89	0.038
39.BD(1)C9-C10	183.RY(1)C4	0.69	1.88	0.032
39.BD(1)C9-C10	184.RY(2)C4	0.81	2.12	0.037
39.BD(1)C9-C10	287.RY(1)C8	0.99	1.94	0.039
40.BD(2)C9-C10	62.LV(1)C4	50.82	0.13	0.072
40.BD(2)C9-C10	78.BD*(2)C7-C8	10.94	0.26	0.048
40.BD(2)C9-C10	185.RY(3)C4	0.69	0.73	0.020
40.BD(2)C9-C10	288.RY(2)C8	1.22	0.73	0.027
41.BD(1)C9-H17	73.BD*(1)C4-C10	4.05	0.89	0.054
41.BD(1)C9-H17	77.BD*(1)C7-C8	3.97	0.95	0.055
41.BD(1)C9-H17	81.BD*(1)C8-H16	0.55	0.79	0.019
41.BD(1)C9-H17	85.BD*(1)C10-H18	0.57	0.77	0.019
41.BD(1)C9-H17	287.RY(1)C8	1.18	1.84	0.042
41.BD(1)C9-H17	339.RY(1)C10	1.30	1.91	0.044
42.BD(1)C10-H18	72.BD*(1)C4-C5	4.63	0.87	0.057
42.BD(1)C10-H18	80.BD*(1)C8-C9	3.85	0.90	0.053
42.BD(1)C10-H18	84.BD*(1)C9-H17	0.57	0.77	0.019
42.BD(1)C10-H18	183.RY(1)C4	0.55	1.78	0.028
42.BD(1)C10-H18	184.RY(2)C4	1.10	2.01	0.042
42.BD(1)C10-H18	313.RY(1)C9	1.21	1.84	0.042
43.BD(1)B14-C21	65.BD*(2)C1-C6	1.37	0.38	0.020
43.BD(1)B14-C21	74.BD*(1)C5-C6	1.98	0.81	0.036
43.BD(1)B14-C21	91.BD*(1)B15-O35	1.16	0.60	0.024
43.BD(1)B14-C21	100.BD*(1)C21-H25	0.61	0.70	0.018
43.BD(1)B14-C21	101.BD*(1)C22-H32	1.69	0.72	0.031
44.BD(1)B14-C22	65.BD*(2)C1-C6	2.69	0.37	0.028
44.BD(1)B14-C22	74.BD*(1)C5-C6	0.97	0.81	0.025
44.BD(1)B14-C22	98.BD*(1)C21-H23	1.83	0.68	0.031
44.BD(1)B14-C22	102.BD*(1)C22-H33	0.53	0.69	0.017
44.BD(1)B14-C22	104.BD*(1)O35-H36	0.81	0.71	0.021
45.BD(1)B14-O35	64.BD*(1)C1-C6	1.20	1.08	0.032
45.BD(1)B14-O35	91.BD*(1)B15-O35	0.64	0.82	0.020
45.BD(1)B14-O35	100.BD*(1)C21-H25	0.95	0.91	0.026
45.BD(1)B14-O35	102.BD*(1)C22-H33	0.88	0.91	0.025

45.BD(1)B14-O35	430.RY(1)B15	1.40	1.62	0.043
45.BD(1)B14-O35	431.RY(2)B15	0.98	1.73	0.037
46.BD(1)B15-C19	75.BD*(1)C5-C7	0.97	0.81	0.025
46.BD(1)B15-C19	78.BD*(2)C7-C8	2.69	0.37	0.028
46.BD(1)B15-C19	94.BD*(1)C19-H28	0.53	0.69	0.017
46.BD(1)B15-C19	95.BD*(1)C20-H29	1.83	0.68	0.031
46.BD(1)B15-C19	104.BD*(1)O35-H36	0.82	0.71	0.021
47.BD(1)B15-C20	75.BD*(1)C5-C7	1.98	0.81	0.036
47.BD(1)B15-C20	78.BD*(2)C7-C8	1.37	0.38	0.020
47.BD(1)B15-C20	88.BD*(1)B14-O35	1.16	0.60	0.024
47.BD(1)B15-C20	92.BD*(1)C19-H26	1.69	0.72	0.031
47.BD(1)B15-C20	96.BD*(1)C20-H30	0.61	0.70	0.018
48.BD(1)B15-O35	77.BD*(1)C7-C8	1.20	1.08	0.032
48.BD(1)B15-O35	88.BD*(1)B14-O35	0.64	0.82	0.020
48.BD(1)B15-O35	94.BD*(1)C19-H28	0.88	0.91	0.025
48.BD(1)B15-O35	96.BD*(1)C20-H30	0.95	0.91	0.026
48.BD(1)B15-O35	404.RY(1)B14	1.40	1.62	0.043
48.BD(1)B15-O35	405.RY(2)B14	0.98	1.73	0.037
49.BD(1)C19-H26	90.BD*(1)B15-C20	1.93	0.73	0.033
49.BD(1)C19-H26	432.RY(3)B15	1.12	1.78	0.040
50.BD(1)C19-H27	79.BD*(1)C7-B15	2.04	0.76	0.035
50.BD(1)C19-H27	91.BD*(1)B15-O35	0.62	0.64	0.018
50.BD(1)C19-H27	434.RY(5)B15	1.14	1.78	0.040
51.BD(1)C19-H28	91.BD*(1)B15-O35	3.22	0.64	0.040
51.BD(1)C19-H28	430.RY(1)B15	0.52	1.44	0.024
51.BD(1)C19-H28	433.RY(4)B15	0.50	2.11	0.029
52.BD(1)C20-H29	89.BD*(1)B15-C19	1.90	0.75	0.034
52.BD(1)C20-H29	91.BD*(1)B15-O35	0.61	0.65	0.018
52.BD(1)C20-H29	432.RY(3)B15	0.78	1.79	0.033
53.BD(1)C20-H30	90.BD*(1)B15-C20	0.53	0.74	0.018
53.BD(1)C20-H30	91.BD*(1)B15-O35	2.57	0.65	0.037
53.BD(1)C20-H30	431.RY(2)B15	0.78	1.56	0.031
54.BD(1)C20-H31	79.BD*(1)C7-B15	2.05	0.78	0.036
54.BD(1)C20-H31	91.BD*(1)B15-O35	0.56	0.65	0.017
54.BD(1)C20-H31	433.RY(4)B15	0.70	2.12	0.034
55.BD(1)C21-H23	87.BD*(1)B14-C22	1.90	0.75	0.034
55.BD(1)C21-H23	88.BD*(1)B14-O35	0.61	0.65	0.018
55.BD(1)C21-H23	406.RY(3)B14	0.78	1.79	0.033
56.BD(1)C21-H24	76.BD*(1)C6-B14	2.05	0.78	0.036
56.BD(1)C21-H24	88.BD*(1)B14-O35	0.56	0.65	0.017
56.BD(1)C21-H24	407.RY(4)B14	0.70	2.12	0.034
57.BD(1)C21-H25	86.BD*(1)B14-C21	0.53	0.74	0.018
57.BD(1)C21-H25	88.BD*(1)B14-O35	2.57	0.65	0.037
57.BD(1)C21-H25	405.RY(2)B14	0.78	1.56	0.031
58.BD(1)C22-H32	86.BD*(1)B14-C21	1.93	0.73	0.033
58.BD(1)C22-H32	406.RY(3)B14	1.12	1.78	0.040
59.BD(1)C22-H33	88.BD*(1)B14-O35	3.22	0.64	0.040
59.BD(1)C22-H33	404.RY(1)B14	0.52	1.44	0.024
59.BD(1)C22-H33	407.RY(4)B14	0.50	2.11	0.029
60.BD(1)C22-H34	76.BD*(1)C6-B14	2.04	0.76	0.035
60.BD(1)C22-H34	88.BD*(1)B14-O35	0.62	0.64	0.018
60.BD(1)C22-H34	408.RY(5)B14	1.14	1.78	0.040
61.BD(1)O35-H36	86.BD*(1)B14-C21	0.66	0.94	0.022
61.BD(1)O35-H36	87.BD*(1)B14-C22	0.85	0.95	0.025
61.BD(1)O35-H36	89.BD*(1)B15-C19	0.85	0.95	0.025
61.BD(1)O35-H36	90.BD*(1)B15-C20	0.65	0.94	0.022
61.BD(1)O35-H36	404.RY(1)B14	2.04	1.65	0.052
61.BD(1)O35-H36	430.RY(1)B15	2.04	1.65	0.052

Table S22. Natural Bond Orbitals Summary for [**1**-OH]$^-$ without Rydberg orbitals.

NBO	Occupancy	Energy / a.u.	Principal delocalizations (geminal,vicinal,remote)
1.CR(1)C1	1.99998	-9.74413	
2.CR(1)C2	1.99998	-9.75747	
3.CR(1)C3	1.99998	-9.75496	
4.CR(1)C4	1.99998	-9.76131	
5.CR(1)C5	1.99998	-9.75460	
6.CR(1)C6	1.99998	-9.72842	
7.CR(1)C7	1.99998	-9.72842	
8.CR(1)C8	1.99998	-9.74413	
9.CR(1)C9	1.99998	-9.75747	
10.CR(1)C10	1.99998	-9.75496	
11.CR(1)B14	1.99996	-6.32648	
12.CR(1)B15	1.99996	-6.32647	
13.CR(1)C19	1.99998	-9.70150	
14.CR(1)C20	1.99998	-9.71338	
15.CR(1)C21	1.99998	-9.71338	
16.CR(1)C22	1.99998	-9.70150	
17.CR(1)O35	1.99999	-18.63593	
18.LP(1)C5	1.00155	0.03805	62(v),65(v),78(v),211(g)
			185(v),68(r),83(r),190(v)
			262(v),236(v),240(v),266(v)
19.LP(1)O35	1.95927	-0.18710	79(v),76(v),87(v),89(v)
			781(v)
20.BD(1)C1-C2	1.98269	-0.38569	71(v),76(v),235(v),64(g)
			67(g),157(v)
21.BD(1)C1-C6	1.97516	-0.37397	75(v),69(v),76(g),209(v)
			63(g),88(v),74(g),407(v)
			210(v),131(v),133(v)
22.BD(2)C1-C6	1.67985	-0.07881	68(v),87(v),132(v),86(v)
			211(v)
23.BD(1)C1-H11	1.97483	-0.28115	74(v),67(v),235(v),131(v)
			69(v),241(v)
24.BD(1)C2-C3	1.98337	-0.40341	73(v),66(v),105(v),63(g)
			70(g),184(v),183(v)
25.BD(2)C2-C3	1.76189	-0.10262	62(v),65(v),106(v),185(v)
26.BD(1)C2-H12	1.97866	-0.30105	70(v),64(v),157(v),105(v)
			71(v),66(v)
27.BD(1)C3-C4	1.97669	-0.38217	69(v),75(v),82(v),209(v)
			339(v),72(g),67(g),73(g)
			131(v),133(v)
28.BD(1)C3-H13	1.97741	-0.30023	72(v),63(v),131(v),184(v)
			69(v),183(v)
29.BD(1)C4-C5	1.96952	-0.36036	71(v),85(v),76(v),79(v)
			235(v),261(v),70(g),73(g)
			74(g),75(g),159(v),341(v)
			238(v),264(v)
30.BD(1)C4-C10	1.97669	-0.38217	84(v),74(v),67(v),209(v)
			157(v),72(g),82(g),70(g)
			313(v),315(v)
31.BD(1)C5-C6	1.97042	-0.35426	66(v),73(v),77(v),183(v)
			75(g),76(g),105(v),261(v)
			72(g),64(g)
32.BD(1)C5-C7	1.97042	-0.35425	81(v),70(v),64(v),183(v)
			74(g),79(g),287(v),235(v)
			72(g),77(g)
33.BD(1)C6-B14	1.95134	-0.21246	63(v),72(v),105(v),210(v)
			103(v),209(v),99(v),66(v)
			64(g),425(g),264(r),235(g)
34.BD(1)C7-C8	1.97517	-0.37398	74(v),84(v),79(g),209(v)
			80(g),91(v),75(g),433(v)
			210(v),313(v),315(v)
35.BD(2)C7-C8	1.67988	-0.07881	83(v),89(v),314(v),90(v)
			211(v)
36.BD(1)C7-B15	1.95134	-0.21246	80(v),72(v),287(v),210(v)
			93(v),209(v),97(v),81(v)
			77(g),451(g),238(r)
37.BD(1)C8-C9	1.98269	-0.38568	85(v),79(v),261(v),77(g)
			82(g),339(v)
38.BD(1)C8-H16	1.97483	-0.28115	75(v),82(v),261(v),313(v)
			84(v),267(v)

39.BD(1)C9-C10	1.98337	-0.40341	70(v),81(v),287(v),80(g)
			73(g),184(v),183(v)
40.BD(2)C9-C10	1.76191	-0.10262	62(v),78(v),288(v),185(v)
41.BD(1)C9-H17	1.97866	-0.30105	73(v),77(v),339(v),287(v)
			85(v),81(v)
42.BD(1)C10-H18	1.97741	-0.30023	72(v),80(v),313(v),184(v)
			84(v),183(v)
43.BD(1)B14-C21	1.96972	-0.21849	74(v),101(v),65(v),91(v)
			100(g)
44.BD(1)B14-C22	1.96218	-0.21096	65(v),98(v),74(v),104(v)
			102(g)
45.BD(1)B14-O35	1.98507	-0.43179	430(v),64(v),431(v),100(v)
			102(v),91(g)
46.BD(1)B15-C19	1.96216	-0.21095	78(v),95(v),75(v),104(v)
			94(g)
47.BD(1)B15-C20	1.96975	-0.21850	75(v),92(v),78(v),88(v)
			96(g)
48.BD(1)B15-O35	1.98506	-0.43178	404(v),77(v),405(v),96(v)
			94(v),88(g)
49.BD(1)C19-H26	1.98686	-0.25007	90(v),432(v)
50.BD(1)C19-H27	1.98556	-0.24997	79(v),434(v),91(v)
51.BD(1)C19-H28	1.98176	-0.25091	91(v),430(v),433(v)
52.BD(1)C20-H29	1.98782	-0.26446	89(v),432(v),91(v)
53.BD(1)C20-H30	1.98386	-0.26399	91(v),431(v),90(g)
54.BD(1)C20-H31	1.98714	-0.26202	79(v),433(v),91(v)
55.BD(1)C21-H23	1.98782	-0.26446	87(v),406(v),88(v)
56.BD(1)C21-H24	1.98714	-0.26203	76(v),407(v),88(v)
57.BD(1)C21-H25	1.98386	-0.26399	88(v),405(v),86(g)
58.BD(1)C22-H32	1.98686	-0.25007	86(v),406(v)
59.BD(1)C22-H33	1.98175	-0.25092	88(v),404(v),407(v)
60.BD(1)C22-H34	1.98556	-0.24997	76(v),408(v),88(v)
61.BD(1)O35-H36	1.98444	-0.46199	430(v),404(v),89(v),87(v)
86(v),90(v)			
------non-Lewis-----			
62.LV(1)C4	0.99666	0.02606	
63.BD*(1)C1-C2	0.01969	0.60417	
64.BD*(1)C1-C6	0.01807	0.64494	
65.BD*(2)C1-C6	0.25667	0.15667	
66.BD*(1)C1-H11	0.02031	0.48544	
67.BD*(1)C2-C3	0.01334	0.63687	
68.BD*(2)C2-C3	0.31223	0.12800	
69.BD*(1)C2-H12	0.01742	0.46687	
70.BD*(1)C3-C4	0.02059	0.58706	
71.BD*(1)C3-H13	0.01859	0.46516	
72.BD*(1)C4-C5	0.03889	0.56549	
73.BD*(1)C4-C10	0.02059	0.58705	
74.BD*(1)C5-C6	0.02918	0.59568	
75.BD*(1)C5-C7	0.02917	0.59566	
76.BD*(1)C6-B14	0.03258	0.51361	
77.BD*(1)C7-C8	0.01807	0.64496	
78.BD*(2)C7-C8	0.25665	0.15667	
79.BD*(1)C7-B15	0.03258	0.51362	
80.BD*(1)C8-C9	0.01969	0.60416	
81.BD*(1)C8-H16	0.02031	0.48545	
82.BD*(1)C9-C10	0.01334	0.63688	
83.BD*(2)C9-C10	0.31220	0.12800	
84.BD*(1)C9-H17	0.01742	0.46687	
85.BD*(1)C10-H18	0.01859	0.46516	
86.BD*(1)B14-C21	0.01792	0.47766	
87.BD*(1)B14-C22	0.02502	0.48504	
88.BD*(1)B14-O35	0.04056	0.38574	
89.BD*(1)B15-C19	0.02502	0.48504	
90.BD*(1)B15-C20	0.01791	0.47768	
91.BD*(1)B15-O35	0.04057	0.38573	
92.BD*(1)C19-H26	0.00739	0.49693	
93.BD*(1)C19-H27	0.00795	0.48259	
94.BD*(1)C19-H28	0.00435	0.48264	
95.BD*(1)C20-H29	0.00775	0.46626	
96.BD*(1)C20-H30	0.00542	0.47657	
97.BD*(1)C20-H31	0.00814	0.47211	
98.BD*(1)C21-H23	0.00775	0.46626	
99.BD*(1)C21-H24	0.00814	0.47209	
100.BD*(1)C21-H25	0.00542	0.47658	

101.BD*(1)C22-H32	0.00740	0.49694	
102.BD*(1)C22-H33	0.00435	0.48263	
103.BD*(1)C22-H34	0.00795	0.48258	
104.BD*(1)O35-H36	0.01188	0.49735	

Table S23. Second order perturbation analysis of the Fock matrix. In NBO-basis for [**1**-SH]$^-$. Threshold for printing the donor acceptor interactions in 0.50 kcal/mol. E(2) is the energy of the donor-acceptor interaction in kcal/mol, E(NL) – E(L) is the energy difference between the donor and acceptor in atomic units and F(L,NL) is the overlap between the donor and acceptor natural orbitals in atomic units.

Donor (L) NBO	Acceptor (NL) NBO	E(2) / kcal/mol	E(NL) – E(L) / a.u	F(L,NL) / a.u.
22.LP(1)S35	80.BD*(1)C6-B14	1.97	0.71	0.034
22.LP(1)S35	83.BD*(1)C7-B15	1.77	0.72	0.032
22.LP(1)S35	408.RY(1)B14	0.81	1.51	0.031
22.LP(1)S35	434.RY(1)B15	0.61	1.48	0.027
23.BD(1)C1-C2	67.BD*(1)C1-C6	1.01	1.02	0.029
23.BD(1)C1-C2	70.BD*(1)C2-C3	0.93	1.03	0.028
23.BD(1)C1-C2	74.BD*(1)C3-H13	2.85	0.85	0.044
23.BD(1)C1-C2	80.BD*(1)C6-B14	2.12	0.87	0.038
23.BD(1)C1-C2	161.RY(1)C3	0.71	2.00	0.034
23.BD(1)C1-C2	239.RY(1)C6	1.48	1.93	0.048
24.BD(1)C1-C6	66.BD*(1)C1-C2	1.01	0.98	0.028
24.BD(1)C1-C6	72.BD*(1)C2-H12	2.28	0.84	0.039
24.BD(1)C1-C6	78.BD*(1)C5-C6	0.68	0.96	0.023
24.BD(1)C1-C6	79.BD*(1)C5-C7	3.64	0.96	0.053
24.BD(1)C1-C6	80.BD*(1)C6-B14	1.43	0.86	0.031
24.BD(1)C1-C6	92.BD*(1)B14-S35	1.41	0.67	0.027
24.BD(1)C1-C6	135.RY(1)C2	0.62	1.92	0.031
24.BD(1)C1-C6	137.RY(3)C2	0.59	1.81	0.029
24.BD(1)C1-C6	213.RY(1)C5	1.08	1.88	0.040
24.BD(1)C1-C6	214.RY(2)C5	0.76	1.96	0.035
25.BD(2)C1-C6	71.BD*(2)C2-C3	17.40	0.21	0.054
25.BD(2)C1-C6	76.BD*(2)C4-C5	13.06	0.22	0.048
25.BD(2)C1-C6	90.BD*(1)B14-C21	2.08	0.54	0.030
25.BD(2)C1-C6	91.BD*(1)B14-C22	2.21	0.54	0.031
25.BD(2)C1-C6	136.RY(2)C2	1.63	0.72	0.030
25.BD(2)C1-C6	215.RY(3)C5	0.67	0.85	0.021
26.BD(1)C1-H11	70.BD*(1)C2-C3	3.72	0.92	0.052
26.BD(1)C1-H11	72.BD*(1)C2-H12	0.63	0.75	0.019
26.BD(1)C1-H11	78.BD*(1)C5-C6	5.25	0.87	0.060
26.BD(1)C1-H11	92.BD*(1)B14-S35	0.74	0.58	0.018
26.BD(1)C1-H11	135.RY(1)C2	1.08	1.83	0.040
26.BD(1)C1-H11	239.RY(1)C6	1.93	1.83	0.053
27.BD(1)C2-C3	66.BD*(1)C1-C2	1.00	1.01	0.028
27.BD(1)C2-C3	69.BD*(1)C1-H11	2.10	0.89	0.039
27.BD(1)C2-C3	73.BD*(1)C3-C4	0.91	0.99	0.027
27.BD(1)C2-C3	77.BD*(1)C4-C10	2.57	0.99	0.045
27.BD(1)C2-C3	109.RY(1)C1	1.05	1.87	0.039
27.BD(1)C2-C3	187.RY(1)C4	0.66	1.85	0.031
27.BD(1)C2-C3	188.RY(2)C4	0.85	2.10	0.038
28.BD(2)C2-C3	68.BD*(2)C1-C6	11.49	0.26	0.049
28.BD(2)C2-C3	76.BD*(2)C4-C5	13.98	0.24	0.052
28.BD(2)C2-C3	110.RY(2)C1	1.08	0.74	0.025
28.BD(2)C2-C3	189.RY(3)C4	0.54	0.77	0.018
29.BD(1)C2-H12	67.BD*(1)C1-C6	4.12	0.94	0.055
29.BD(1)C2-H12	69.BD*(1)C1-H11	0.56	0.79	0.019
29.BD(1)C2-H12	73.BD*(1)C3-C4	3.99	0.89	0.053
29.BD(1)C2-H12	74.BD*(1)C3-H13	0.56	0.77	0.018
29.BD(1)C2-H12	109.RY(1)C1	1.12	1.77	0.040
29.BD(1)C2-H12	161.RY(1)C3	1.26	1.91	0.044
30.BD(1)C3-C4	70.BD*(1)C2-C3	0.86	1.02	0.026
30.BD(1)C3-C4	72.BD*(1)C2-H12	2.79	0.85	0.043
30.BD(1)C3-C4	75.BD*(1)C4-C5	0.83	0.94	0.025
30.BD(1)C3-C4	77.BD*(1)C4-C10	0.72	0.97	0.023
30.BD(1)C3-C4	79.BD*(1)C5-C7	2.55	0.97	0.044
30.BD(1)C3-C4	86.BD*(1)C9-C10	2.00	1.02	0.040

30.BD(1)C3-C4	135.RY(1)C2	0.68	1.93	0.032
30.BD(1)C3-C4	137.RY(3)C2	0.59	1.82	0.029
30.BD(1)C3-C4	213.RY(1)C5	1.21	1.89	0.043
30.BD(1)C3-C4	343.RY(1)C10	0.99	1.99	0.040
31.BD(1)C3-H13	66.BD*(1)C1-C2	3.79	0.91	0.052
31.BD(1)C3-H13	72.BD*(1)C2-H12	0.57	0.77	0.019
31.BD(1)C3-H13	75.BD*(1)C4-C5	4.72	0.86	0.057
31.BD(1)C3-H13	135.RY(1)C2	1.20	1.85	0.042
31.BD(1)C3-H13	187.RY(1)C4	0.51	1.75	0.027
31.BD(1)C3-H13	188.RY(2)C4	1.11	2.00	0.042
32.BD(1)C4-C5	73.BD*(1)C3-C4	0.68	0.95	0.023
32.BD(1)C4-C5	74.BD*(1)C3-H13	2.39	0.83	0.040
32.BD(1)C4-C5	77.BD*(1)C4-C10	0.66	0.94	0.022
32.BD(1)C4-C5	78.BD*(1)C5-C6	0.66	0.95	0.022
32.BD(1)C4-C5	79.BD*(1)C5-C7	0.61	0.94	0.021
32.BD(1)C4-C5	80.BD*(1)C6-B14	2.63	0.85	0.042
32.BD(1)C4-C5	83.BD*(1)C7-B15	2.44	0.85	0.041
32.BD(1)C4-C5	89.BD*(1)C10-H18	2.36	0.83	0.039
32.BD(1)C4-C5	163.RY(3)C3	0.55	1.92	0.029
32.BD(1)C4-C5	239.RY(1)C6	0.83	1.91	0.035
32.BD(1)C4-C5	265.RY(1)C7	0.78	1.92	0.035
32.BD(1)C4-C5	345.RY(3)C10	0.52	1.85	0.028
33.BD(2)C4-C5	68.BD*(2)C1-C6	15.15	0.23	0.053
33.BD(2)C4-C5	71.BD*(2)C2-C3	15.26	0.20	0.050
33.BD(2)C4-C5	82.BD*(2)C7-C8	14.91	0.23	0.052
33.BD(2)C4-C5	87.BD*(2)C9-C10	15.16	0.20	0.050
33.BD(2)C4-C5	162.RY(2)C3	1.05	0.72	0.025
33.BD(2)C4-C5	344.RY(2)C10	0.96	0.77	0.024
34.BD(1)C4-C10	70.BD*(1)C2-C3	2.02	1.02	0.040
34.BD(1)C4-C10	73.BD*(1)C3-C4	0.71	0.97	0.023
34.BD(1)C4-C10	75.BD*(1)C4-C5	0.82	0.94	0.025
34.BD(1)C4-C10	78.BD*(1)C5-C6	2.61	0.97	0.045
34.BD(1)C4-C10	86.BD*(1)C9-C10	0.85	1.02	0.026
34.BD(1)C4-C10	88.BD*(1)C9-H17	2.81	0.85	0.044
34.BD(1)C4-C10	161.RY(1)C3	0.99	1.99	0.040
34.BD(1)C4-C10	213.RY(1)C5	1.26	1.88	0.043
34.BD(1)C4-C10	317.RY(1)C9	0.67	1.94	0.032
34.BD(1)C4-C10	319.RY(3)C9	0.61	1.80	0.029
35.BD(1)C5-C6	67.BD*(1)C1-C6	0.56	0.99	0.021
35.BD(1)C5-C6	69.BD*(1)C1-H11	3.18	0.84	0.046
35.BD(1)C5-C6	75.BD*(1)C4-C5	0.64	0.92	0.022
35.BD(1)C5-C6	77.BD*(1)C4-C10	2.67	0.94	0.045
35.BD(1)C5-C6	79.BD*(1)C5-C7	1.04	0.94	0.028
35.BD(1)C5-C6	80.BD*(1)C6-B14	0.79	0.84	0.023
35.BD(1)C5-C6	81.BD*(1)C7-C8	2.45	1.00	0.044
35.BD(1)C5-C6	109.RY(1)C1	0.75	1.82	0.033
35.BD(1)C5-C6	187.RY(1)C4	1.19	1.80	0.041
35.BD(1)C5-C6	265.RY(1)C7	0.74	1.92	0.034
36.BD(1)C5-C7	67.BD*(1)C1-C6	2.38	0.99	0.043
36.BD(1)C5-C7	73.BD*(1)C3-C4	2.74	0.94	0.045
36.BD(1)C5-C7	75.BD*(1)C4-C5	0.61	0.91	0.021
36.BD(1)C5-C7	78.BD*(1)C5-C6	1.01	0.94	0.028
36.BD(1)C5-C7	83.BD*(1)C7-B15	0.82	0.85	0.024
36.BD(1)C5-C7	85.BD*(1)C8-H16	3.21	0.85	0.047
36.BD(1)C5-C7	187.RY(1)C4	1.14	1.80	0.040
36.BD(1)C5-C7	239.RY(1)C6	0.65	1.90	0.032
36.BD(1)C5-C7	291.RY(1)C8	0.77	1.87	0.034
36.BD(1)C5-C7	434.RY(1)B15	0.55	1.61	0.027
37.BD(1)C6-B14	66.BD*(1)C1-C2	5.03	0.83	0.058
37.BD(1)C6-B14	67.BD*(1)C1-C6	0.59	0.85	0.020
37.BD(1)C6-B14	69.BD*(1)C1-H11	0.71	0.70	0.020
37.BD(1)C6-B14	75.BD*(1)C4-C5	3.81	0.78	0.049
37.BD(1)C6-B14	103.BD*(1)C21-H27	1.52	0.70	0.029
37.BD(1)C6-B14	107.BD*(1)C22-H31	1.54	0.70	0.029
37.BD(1)C6-B14	109.RY(1)C1	1.64	1.68	0.047
37.BD(1)C6-B14	213.RY(1)C5	1.26	1.72	0.042
37.BD(1)C6-B14	214.RY(2)C5	1.79	1.81	0.051
38.BD(1)C7-C8	78.BD*(1)C5-C6	3.57	0.96	0.052
38.BD(1)C7-C8	79.BD*(1)C5-C7	0.66	0.96	0.023
38.BD(1)C7-C8	83.BD*(1)C7-B15	1.44	0.87	0.032
38.BD(1)C7-C8	84.BD*(1)C8-C9	1.03	0.98	0.028
38.BD(1)C7-C8	88.BD*(1)C9-H17	2.23	0.84	0.039
38.BD(1)C7-C8	95.BD*(1)B15-S35	0.81	0.67	0.021

38.BD(1)C7-C8	213.RY(1)C5	1.29	1.88	0.044
38.BD(1)C7-C8	214.RY(2)C5	0.54	1.96	0.029
38.BD(1)C7-C8	317.RY(1)C9	0.62	1.93	0.031
38.BD(1)C7-C8	319.RY(3)C9	0.52	1.79	0.027
39.BD(2)C7-C8	76.BD*(2)C4-C5	12.70	0.22	0.047
39.BD(2)C7-C8	87.BD*(2)C9-C10	16.98	0.21	0.053
39.BD(2)C7-C8	93.BD*(1)B15-C19	3.08	0.54	0.036
39.BD(2)C7-C8	95.BD*(1)B15-S35	2.60	0.37	0.028
39.BD(2)C7-C8	215.RY(3)C5	0.92	0.85	0.025
39.BD(2)C7-C8	318.RY(2)C9	1.56	0.72	0.030
40.BD(1)C7-B15	75.BD*(1)C4-C5	3.83	0.78	0.049
40.BD(1)C7-B15	81.BD*(1)C7-C8	0.59	0.86	0.020
40.BD(1)C7-B15	84.BD*(1)C8-C9	4.78	0.82	0.056
40.BD(1)C7-B15	85.BD*(1)C8-H16	0.72	0.71	0.020
40.BD(1)C7-B15	97.BD*(1)C19-H24	1.70	0.70	0.031
40.BD(1)C7-B15	101.BD*(1)C20-H34	1.26	0.70	0.027
40.BD(1)C7-B15	213.RY(1)C5	1.52	1.72	0.046
40.BD(1)C7-B15	214.RY(2)C5	1.52	1.81	0.047
40.BD(1)C7-B15	291.RY(1)C8	1.82	1.74	0.050
41.BD(1)C8-C9	81.BD*(1)C7-C8	1.00	1.03	0.029
41.BD(1)C8-C9	83.BD*(1)C7-B15	2.17	0.88	0.039
41.BD(1)C8-C9	86.BD*(1)C9-C10	0.91	1.03	0.027
41.BD(1)C8-C9	89.BD*(1)C10-H18	2.89	0.85	0.044
41.BD(1)C8-C9	265.RY(1)C7	1.49	1.95	0.048
41.BD(1)C8-C9	343.RY(1)C10	0.72	1.99	0.034
42.BD(1)C8-H16	79.BD*(1)C5-C7	5.28	0.86	0.060
42.BD(1)C8-H16	86.BD*(1)C9-C10	3.68	0.92	0.052
42.BD(1)C8-H16	88.BD*(1)C9-H17	0.62	0.75	0.019
42.BD(1)C8-H16	101.BD*(1)C20-H34	0.54	0.76	0.018
42.BD(1)C8-H16	265.RY(1)C7	1.89	1.84	0.053
42.BD(1)C8-H16	317.RY(1)C9	1.07	1.83	0.040
43.BD(1)C9-C10	73.BD*(1)C3-C4	2.53	0.99	0.045
43.BD(1)C9-C10	77.BD*(1)C4-C10	0.91	0.99	0.027
43.BD(1)C9-C10	84.BD*(1)C8-C9	0.96	1.01	0.028
43.BD(1)C9-C10	85.BD*(1)C8-H16	2.03	0.90	0.038
43.BD(1)C9-C10	187.RY(1)C4	0.74	1.85	0.033
43.BD(1)C9-C10	188.RY(2)C4	0.79	2.10	0.036
43.BD(1)C9-C10	291.RY(1)C8	1.00	1.92	0.039
44.BD(2)C9-C10	76.BD*(2)C4-C5	13.72	0.24	0.052
44.BD(2)C9-C10	82.BD*(2)C7-C8	11.28	0.26	0.048
44.BD(2)C9-C10	189.RY(3)C4	0.58	0.77	0.019
44.BD(2)C9-C10	292.RY(2)C8	1.14	0.74	0.026
45.BD(1)C9-H17	77.BD*(1)C4-C10	4.07	0.89	0.054
45.BD(1)C9-H17	81.BD*(1)C7-C8	4.06	0.95	0.055
45.BD(1)C9-H17	85.BD*(1)C8-H16	0.53	0.79	0.018
45.BD(1)C9-H17	89.BD*(1)C10-H18	0.56	0.77	0.019
45.BD(1)C9-H17	291.RY(1)C8	1.16	1.82	0.041
45.BD(1)C9-H17	343.RY(1)C10	1.28	1.91	0.044
46.BD(1)C10-H18	75.BD*(1)C4-C5	4.70	0.86	0.057
46.BD(1)C10-H18	84.BD*(1)C8-C9	3.82	0.90	0.052
46.BD(1)C10-H18	88.BD*(1)C9-H17	0.57	0.77	0.019
46.BD(1)C10-H18	187.RY(1)C4	0.57	1.75	0.028
46.BD(1)C10-H18	188.RY(2)C4	1.07	2.00	0.041
46.BD(1)C10-H18	317.RY(1)C9	1.22	1.85	0.043
47.BD(1)B14-C21	68.BD*(2)C1-C6	2.00	0.38	0.024
47.BD(1)B14-C21	78.BD*(1)C5-C6	1.92	0.81	0.035
47.BD(1)B14-C21	103.BD*(1)C21-H27	0.52	0.70	0.017
47.BD(1)B14-C21	105.BD*(1)C22-H29	1.83	0.72	0.032
48.BD(1)B14-C22	68.BD*(2)C1-C6	1.81	0.37	0.023
48.BD(1)B14-C22	78.BD*(1)C5-C6	1.72	0.81	0.033
48.BD(1)B14-C22	102.BD*(1)C21-H26	1.81	0.70	0.032
48.BD(1)B14-C22	105.BD*(1)C22-H29	0.51	0.72	0.017
48.BD(1)B14-C22	107.BD*(1)C22-H31	0.51	0.70	0.017
48.BD(1)B14-C22	108.BD*(1)S35-H36	0.96	0.50	0.019
49.BD(1)B14-S35	67.BD*(1)C1-C6	2.07	0.88	0.038
49.BD(1)B14-S35	94.BD*(1)B15-C20	1.30	0.72	0.027
49.BD(1)B14-S35	104.BD*(1)C21-H28	2.26	0.73	0.036
49.BD(1)B14-S35	106.BD*(1)C22-H30	2.11	0.73	0.035
49.BD(1)B14-S35	577.RY(1)C22	0.65	1.24	0.025
50.BD(1)B15-C19	81.BD*(1)C7-C8	0.58	0.86	0.020
50.BD(1)B15-C19	82.BD*(2)C7-C8	3.56	0.37	0.032
50.BD(1)B15-C19	96.BD*(1)C19-H23	0.51	0.72	0.017
50.BD(1)B15-C19	99.BD*(1)C20-H32	1.90	0.70	0.032

50.BD(1)B15-C19	108.BD*(1)S35-H36	0.95	0.49	0.019
50.BD(1)B15-C19	761.RY(3)S35	0.54	1.26	0.023
51.BD(1)B15-C20	79.BD*(1)C5-C7	2.84	0.81	0.043
51.BD(1)B15-C20	92.BD*(1)B14-S35	0.56	0.52	0.015
51.BD(1)B15-C20	96.BD*(1)C19-H23	1.67	0.72	0.031
51.BD(1)B15-C20	101.BD*(1)C20-H34	0.59	0.71	0.018
52.BD(1)B15-S35	81.BD*(1)C7-C8	1.90	0.89	0.037
52.BD(1)B15-S35	82.BD*(2)C7-C8	0.91	0.40	0.017
52.BD(1)B15-S35	90.BD*(1)B14-C21	1.05	0.71	0.024
52.BD(1)B15-S35	98.BD*(1)C19-H25	1.97	0.73	0.034
52.BD(1)B15-S35	100.BD*(1)C20-H33	2.33	0.72	0.037
52.BD(1)B15-S35	499.RY(1)C19	0.63	1.26	0.025
53.BD(1)C19-H23	94.BD*(1)B15-C20	1.98	0.72	0.034
53.BD(1)C19-H23	435.RY(2)B15	0.92	1.52	0.033
54.BD(1)C19-H24	83.BD*(1)C7-B15	2.05	0.75	0.035
54.BD(1)C19-H24	438.RY(5)B15	0.59	1.96	0.030
55.BD(1)C19-H25	93.BD*(1)B15-C19	0.78	0.71	0.021
55.BD(1)C19-H25	95.BD*(1)B15-S35	3.34	0.54	0.038
55.BD(1)C19-H25	437.RY(4)B15	0.59	2.08	0.031
56.BD(1)C20-H32	93.BD*(1)B15-C19	2.10	0.72	0.035
56.BD(1)C20-H32	435.RY(2)B15	0.98	1.53	0.035
57.BD(1)C20-H33	94.BD*(1)B15-C20	0.64	0.73	0.019
57.BD(1)C20-H33	95.BD*(1)B15-S35	2.80	0.55	0.035
58.BD(1)C20-H34	83.BD*(1)C7-B15	2.55	0.75	0.039
58.BD(1)C20-H34	94.BD*(1)B15-C20	0.56	0.73	0.018
58.BD(1)C20-H34	434.RY(1)B15	0.55	1.51	0.026
58.BD(1)C20-H34	437.RY(4)B15	0.54	2.09	0.030
59.BD(1)C21-H26	91.BD*(1)B14-C22	2.05	0.72	0.034
59.BD(1)C21-H26	409.RY(2)B14	0.91	1.51	0.033
60.BD(1)C21-H27	80.BD*(1)C6-B14	2.25	0.74	0.037
61.BD(1)C21-H28	90.BD*(1)B14-C21	0.67	0.72	0.020
61.BD(1)C21-H28	92.BD*(1)B14-S35	2.66	0.55	0.034
62.BD(1)C22-H29	90.BD*(1)B14-C21	1.96	0.72	0.033
62.BD(1)C22-H29	409.RY(2)B14	1.06	1.51	0.036
63.BD(1)C22-H30	91.BD*(1)B14-C22	0.73	0.71	0.020
63.BD(1)C22-H30	92.BD*(1)B14-S35	3.18	0.55	0.037
64.BD(1)C22-H31	80.BD*(1)C6-B14	2.37	0.74	0.037
64.BD(1)C22-H31	410.RY(3)B14	0.91	1.43	0.032
65.BD(1)S35-H36	91.BD*(1)B14-C22	1.50	0.77	0.030
65.BD(1)S35-H36	93.BD*(1)B15-C19	1.71	0.77	0.032

Table S24. Natural Bond Orbitals Summary for [**1**-SH]$^-$ without Rydberg orbitals.

NBO	Occupancy	Energy / a.u.	Principal delocalizations (geminal,vicinal,remote)
1.CR(1)C1	1.99998	-9.74752	
2.CR(1)C2	1.99998	-9.75971	
3.CR(1)C3	1.99998	-9.75784	
4.CR(1)C4	1.99998	-9.76479	
5.CR(1)C5	1.99998	-9.76069	
6.CR(1)C6	1.99998	-9.73728	
7.CR(1)C7	1.99998	-9.73562	
8.CR(1)C8	1.99998	-9.74642	
9.CR(1)C9	1.99998	-9.75956	
10.CR(1)C10	1.99998	-9.75828	
11.CR(1)B14	1.99996	-6.32570	
12.CR(1)B15	1.99996	-6.32324	
13.CR(1)C19	1.99998	-9.71001	
14.CR(1)C20	1.99998	-9.71424	
15.CR(1)C21	1.99998	-9.71508	
16.CR(1)C22	1.99998	-9.71139	
17.CR(1)S35	2.00000	-84.10514	
18.CR(2)S35	1.99998	-11.33999	
19.CR(3)S35	1.99999	-5.55095	
20.CR(4)S35	1.99999	-5.55290	
21.CR(5)S35	1.99999	-5.55750	
22.LP(1)S35	1.97305	-0.23091	80(v),83(v),408(v),434(v)
23.BD(1)C1-C2	1.98192	-0.38955	74(v),80(v),239(v),67(g)
			70(g),161(v)
24.BD(1)C1-C6	1.97194	-0.37540	79(v),72(v),80(g),92(v)
			213(v),66(g),214(v),78(g)
			135(v),137(v)
25.BD(2)C1-C6	1.67787	-0.08186	71(v),76(v),91(v),90(v)
			136(v),215(v)
26.BD(1)C1-H11	1.97298	-0.28329	78(v),70(v),239(v),135(v)
			92(r),72(v)
27.BD(1)C2-C3	1.98327	-0.40638	77(v),69(v),109(v),66(g)
			73(g),188(v),187(v)
28.BD(2)C2-C3	1.75614	-0.10551	76(v),68(v),110(v),189(v)
29.BD(1)C2-H12	1.97838	-0.30388	67(v),73(v),161(v),109(v)
			69(v),74(v)
30.BD(1)C3-C4	1.97630	-0.38524	72(v),79(v),86(v),213(v)
			343(v),70(g),75(g),77(g)
			135(v),137(v)
31.BD(1)C3-H13	1.97712	-0.30324	75(v),66(v),135(v),188(v)
			72(v),187(v)
32.BD(1)C4-C5	1.96812	-0.36277	80(v),83(v),74(v),89(v)
			239(v),265(v),73(g),77(g)
			78(g),79(g),163(v),345(v)
33.BD(2)C4-C5	1.52122	-0.07886	71(v),87(v),68(v),82(v)
			162(v),344(v)
34.BD(1)C4-C10	1.97614	-0.38446	88(v),78(v),70(v),213(v)
			161(v),86(g),75(g),73(g)
			317(v),319(v)
35.BD(1)C5-C6	1.97184	-0.35967	69(v),77(v),81(v),187(v)
			79(g),80(g),109(v),265(v)
			75(g),67(g)
36.BD(1)C5-C7	1.97142	-0.35628	85(v),73(v),67(v),187(v)
			78(g),83(g),291(v),239(v)
			75(g),434(v)
37.BD(1)C6-B14	1.94935	-0.22059	66(v),75(v),214(v),109(v)
			107(v),103(v),213(v),69(v)
			67(g)
38.BD(1)C7-C8	1.97368	-0.37698	78(v),88(v),83(g),213(v)
			84(g),95(v),79(g),317(v)
			214(v),319(v)
39.BD(2)C7-C8	1.69139	-0.08274	87(v),76(v),93(v),95(v)
			318(v),215(v)
40.BD(1)C7-B15	1.95010	-0.22164	84(v),75(v),291(v),97(v)
			213(v),214(v),101(v),85(v)
			81(g)
41.BD(1)C8-C9	1.98202	-0.38732	89(v),83(v),265(v),81(g)
			86(g),343(v)
42.BD(1)C8-H16	1.97335	-0.28209	79(v),86(v),265(v),317(v)

			88(v),101(r)
43.BD(1)C9-C10	1.98365	-0.40754	73(v),85(v),291(v),84(g)
			77(g),188(v),187(v)
44.BD(2)C9-C10	1.76580	-0.10624	76(v),82(v),292(v),189(v)
45.BD(1)C9-H17	1.97853	-0.30385	77(v),81(v),343(v),291(v)
			89(v),85(v)
46.BD(1)C10-H18	1.97711	-0.30334	75(v),84(v),317(v),188(v)
			88(v),187(v)
47.BD(1)B14-C21	1.96191	-0.22317	68(v),78(v),105(v),103(g)
48.BD(1)B14-C22	1.96243	-0.22280	102(v),68(v),78(v),108(v)
			107(g),105(g)
49.BD(1)B14-S35	1.97021	-0.25233	104(v),106(v),67(v),94(v)
			577(v)
50.BD(1)B15-C19	1.95503	-0.21995	82(v),99(v),108(v),81(v)
			761(v),96(g)
51.BD(1)B15-C20	1.97377	-0.22571	79(v),96(v),101(g),92(v)
52.BD(1)B15-S35	1.96520	-0.24778	100(v),98(v),81(v),90(v)
			82(v),499(v)
53.BD(1)C19-H23	1.98681	-0.25526	94(v),435(v)
54.BD(1)C19-H24	1.98533	-0.25667	83(v),438(v)
55.BD(1)C19-H25	1.97985	-0.25449	95(v),93(g),437(v)
56.BD(1)C20-H32	1.98861	-0.26185	93(v),435(v)
57.BD(1)C20-H33	1.98196	-0.26223	95(v),94(g)
58.BD(1)C20-H34	1.98642	-0.26011	83(v),94(g),434(v),437(v)
59.BD(1)C21-H26	1.98826	-0.26100	91(v),409(v)
60.BD(1)C21-H27	1.98560	-0.26082	80(v)
61.BD(1)C21-H28	1.98142	-0.26145	92(v),90(g)
62.BD(1)C22-H29	1.98743	-0.25756	90(v),409(v)
63.BD(1)C22-H30	1.97970	-0.25748	92(v),91(g)
64.BD(1)C22-H31	1.98641	-0.25701	80(v),410(v)
65.BD(1)S35-H36	1.98531	-0.31452	93(v),91(v)
------non-LewiS---------			
66.BD*(1)C1-C2	0.02025	0.60623	
67.BD*(1)C1-C6	0.01971	0.63265	
68.BD*(2)C1-C6	0.25864	0.15198	
69.BD*(1)C1-H11	0.02057	0.48377	
70.BD*(1)C2-C3	0.01351	0.63634	
71.BD*(2)C2-C3	0.31322	0.12565	
72.BD*(1)C2-H12	0.01772	0.46428	
73.BD*(1)C3-C4	0.02040	0.58452	
74.BD*(1)C3-H13	0.01859	0.46292	
75.BD*(1)C4-C5	0.03860	0.55849	
76.BD*(2)C4-C5	0.47216	0.13748	
77.BD*(1)C4-C10	0.02057	0.58141	
78.BD*(1)C5-C6	0.03066	0.58659	
79.BD*(1)C5-C7	0.03011	0.58159	
80.BD*(1)C6-B14	0.03532	0.48348	
81.BD*(1)C7-C8	0.02006	0.64162	
82.BD*(2)C7-C8	0.25604	0.15239	
83.BD*(1)C7-B15	0.03358	0.49162	
84.BD*(1)C8-C9	0.02017	0.60099	
85.BD*(1)C8-H16	0.02037	0.49021	
86.BD*(1)C9-C10	0.01341	0.63897	
87.BD*(2)C9-C10	0.30151	0.12575	
88.BD*(1)C9-H17	0.01768	0.46446	
89.BD*(1)C10-H18	0.01864	0.46283	
90.BD*(1)B14-C21	0.02134	0.45816	
91.BD*(1)B14-C22	0.02327	0.45734	
92.BD*(1)B14-S35	0.04132	0.29225	
93.BD*(1)B15-C19	0.02450	0.45881	
94.BD*(1)B15-C20	0.01898	0.46709	
95.BD*(1)B15-S35	0.04830	0.29007	
96.BD*(1)C19-H23	0.00733	0.49835	
97.BD*(1)C19-H24	0.00818	0.47954	
98.BD*(1)C19-H25	0.00785	0.47864	
99.BD*(1)C20-H32	0.00772	0.47581	
100.BD*(1)C20-H33	0.01016	0.47179	
101.BD*(1)C20-H34	0.00732	0.48145	
102.BD*(1)C21-H26	0.00754	0.47706	
103.BD*(1)C21-H27	0.00813	0.47634	
104.BD*(1)C21-H28	0.01003	0.47570	
105.BD*(1)C22-H29	0.00791	0.49386	
106.BD*(1)C22-H30	0.00832	0.47635	

107.BD*(1)C22-H31	0.00814	0.47800	
108.BD*(1)S35-H36	0.02263	0.27423	

Table S25. Second order perturbation analysis of the Fock matrix. In NBO-basis for [**1**-SeH]⁻. Threshold for printing the donor acceptor interactions in 0.50 kcal/mol. E(2) is the energy of the donor-acceptor interaction in kcal/mol, E(NL) – E(L) is the energy difference between the donor and acceptor in atomic units and F(L,NL) is the overlap between the donor and acceptor natural orbitals in atomic units.

Donor (L) NBO	Acceptor (NL) NBO	E(2) / kcal/mol	E(NL) – E(L) / a.u	F(L,NL) / a.u.
31.LP(1)Se35	89.BD*(1)C6-B14	1.42	0.73	0.029
31.LP(1)Se35	92.BD*(1)C7-B15	1.12	0.74	0.026
31.LP(1)Se35	417.RY(1)B14	0.81	1.51	0.031
32.BD(1)C1-C2	76.BD*(1)C1-C6	1.02	1.02	0.029
32.BD(1)C1-C2	79.BD*(1)C2-C3	0.94	1.03	0.028
32.BD(1)C1-C2	83.BD*(1)C3-H13	2.86	0.85	0.044
32.BD(1)C1-C2	89.BD*(1)C6-B14	2.22	0.87	0.039
32.BD(1)C1-C2	170.RY(1)C3	0.70	2.00	0.034
32.BD(1)C1-C2	248.RY(1)C6	1.47	1.87	0.047
33.BD(1)C1-C6	75.BD*(1)C1-C2	1.02	0.98	0.028
33.BD(1)C1-C6	81.BD*(1)C2-H12	2.27	0.84	0.039
33.BD(1)C1-C6	87.BD*(1)C5-C6	0.68	0.96	0.023
33.BD(1)C1-C6	88.BD*(1)C5-C7	3.68	0.95	0.053
33.BD(1)C1-C6	89.BD*(1)C6-B14	1.51	0.85	0.032
33.BD(1)C1-C6	101.BD*(1)B14-Se35	1.88	0.62	0.031
33.BD(1)C1-C6	144.RY(1)C2	0.62	1.92	0.031
33.BD(1)C1-C6	146.RY(3)C2	0.60	1.82	0.030
33.BD(1)C1-C6	222.RY(1)C5	0.96	1.83	0.037
33.BD(1)C1-C6	223.RY(2)C5	0.82	1.91	0.035
34.BD(2)C1-C6	80.BD*(2)C2-C3	17.27	0.21	0.053
34.BD(2)C1-C6	85.BD*(2)C4-C5	12.88	0.22	0.047
34.BD(2)C1-C6	99.BD*(1)B14-C21	2.31	0.54	0.032
34.BD(2)C1-C6	100.BD*(1)B14-C22	2.12	0.54	0.030
34.BD(2)C1-C6	112.BD*(1)C21-H27	0.51	0.56	0.015
34.BD(2)C1-C6	145.RY(2)C2	1.64	0.72	0.031
34.BD(2)C1-C6	224.RY(3)C5	0.74	0.84	0.022
35.BD(1)C1-H11	79.BD*(1)C2-C3	3.70	0.92	0.052
35.BD(1)C1-H11	81.BD*(1)C2-H12	0.63	0.75	0.019
35.BD(1)C1-H11	87.BD*(1)C5-C6	5.14	0.87	0.060
35.BD(1)C1-H11	101.BD*(1)B14-Se35	1.04	0.53	0.021
35.BD(1)C1-H11	144.RY(1)C2	1.08	1.83	0.040
35.BD(1)C1-H11	248.RY(1)C6	1.85	1.76	0.051
36.BD(1)C2-C3	75.BD*(1)C1-C2	1.01	1.01	0.029
36.BD(1)C2-C3	78.BD*(1)C1-H11	2.09	0.89	0.039
36.BD(1)C2-C3	82.BD*(1)C3-C4	0.91	0.99	0.027
36.BD(1)C2-C3	86.BD*(1)C4-C10	2.55	0.99	0.045
36.BD(1)C2-C3	118.RY(1)C1	1.05	1.84	0.039
36.BD(1)C2-C3	196.RY(1)C4	0.69	1.84	0.032
36.BD(1)C2-C3	197.RY(2)C4	0.85	2.09	0.038
37.BD(2)C2-C3	77.BD*(2)C1-C6	11.66	0.26	0.049
37.BD(2)C2-C3	85.BD*(2)C4-C5	13.96	0.24	0.052
37.BD(2)C2-C3	119.RY(2)C1	1.05	0.74	0.025
37.BD(2)C2-C3	198.RY(3)C4	0.54	0.77	0.018
38.BD(1)C2-H12	76.BD*(1)C1-C6	4.15	0.93	0.056
38.BD(1)C2-H12	78.BD*(1)C1-H11	0.56	0.79	0.019
38.BD(1)C2-H12	82.BD*(1)C3-C4	3.98	0.89	0.053
38.BD(1)C2-H12	83.BD*(1)C3-H13	0.55	0.77	0.018
38.BD(1)C2-H12	118.RY(1)C1	1.08	1.74	0.039
38.BD(1)C2-H12	170.RY(1)C3	1.25	1.91	0.044
39.BD(1)C3-C4	79.BD*(1)C2-C3	0.86	1.02	0.026
39.BD(1)C3-C4	81.BD*(1)C2-H12	2.80	0.85	0.044
39.BD(1)C3-C4	84.BD*(1)C4-C5	0.83	0.94	0.025
39.BD(1)C3-C4	86.BD*(1)C4-C10	0.71	0.97	0.023
39.BD(1)C3-C4	88.BD*(1)C5-C7	2.53	0.96	0.044
39.BD(1)C3-C4	95.BD*(1)C9-C10	2.01	1.02	0.041
39.BD(1)C3-C4	144.RY(1)C2	0.68	1.93	0.032
39.BD(1)C3-C4	146.RY(3)C2	0.60	1.83	0.029
39.BD(1)C3-C4	222.RY(1)C5	1.18	1.84	0.042
39.BD(1)C3-C4	352.RY(1)C10	0.99	1.99	0.040
40.BD(1)C3-H13	75.BD*(1)C1-C2	3.78	0.91	0.052
40.BD(1)C3-H13	81.BD*(1)C2-H12	0.57	0.77	0.019
40.BD(1)C3-H13	84.BD*(1)C4-C5	4.74	0.86	0.057
40.BD(1)C3-H13	144.RY(1)C2	1.20	1.85	0.042

40.BD(1)C3-H13	196.RY(1)C4	0.52	1.74	0.027
40.BD(1)C3-H13	197.RY(2)C4	1.10	1.99	0.042
41.BD(1)C4-C5	82.BD*(1)C3-C4	0.68	0.95	0.023
41.BD(1)C4-C5	83.BD*(1)C3-H13	2.38	0.83	0.040
41.BD(1)C4-C5	86.BD*(1)C4-C10	0.65	0.94	0.022
41.BD(1)C4-C5	87.BD*(1)C5-C6	0.66	0.95	0.022
41.BD(1)C4-C5	88.BD*(1)C5-C7	0.59	0.94	0.021
41.BD(1)C4-C5	89.BD*(1)C6-B14	2.77	0.84	0.043
41.BD(1)C4-C5	92.BD*(1)C7-B15	2.54	0.85	0.042
41.BD(1)C4-C5	98.BD*(1)C10-H18	2.34	0.83	0.039
41.BD(1)C4-C5	172.RY(3)C3	0.55	1.89	0.029
41.BD(1)C4-C5	248.RY(1)C6	0.84	1.84	0.035
41.BD(1)C4-C5	274.RY(1)C7	0.78	1.86	0.034
41.BD(1)C4-C5	354.RY(3)C10	0.51	1.82	0.027
42.BD(2)C4-C5	77.BD*(2)C1-C6	14.99	0.23	0.052
42.BD(2)C4-C5	80.BD*(2)C2-C3	15.32	0.20	0.050
42.BD(2)C4-C5	91.BD*(2)C7-C8	14.66	0.23	0.052
42.BD(2)C4-C5	96.BD*(2)C9-C10	15.20	0.20	0.050
42.BD(2)C4-C5	171.RY(2)C3	0.99	0.74	0.024
42.BD(2)C4-C5	224.RY(3)C5	0.54	0.83	0.019
42.BD(2)C4-C5	353.RY(2)C10	0.91	0.79	0.024
43.BD(1)C4-C10	79.BD*(1)C2-C3	2.03	1.02	0.041
43.BD(1)C4-C10	82.BD*(1)C3-C4	0.71	0.97	0.023
43.BD(1)C4-C10	84.BD*(1)C4-C5	0.82	0.94	0.025
43.BD(1)C4-C10	87.BD*(1)C5-C6	2.62	0.97	0.045
43.BD(1)C4-C10	95.BD*(1)C9-C10	0.85	1.02	0.026
43.BD(1)C4-C10	97.BD*(1)C9-H17	2.82	0.85	0.044
43.BD(1)C4-C10	170.RY(1)C3	1.00	1.99	0.040
43.BD(1)C4-C10	222.RY(1)C5	1.25	1.84	0.043
43.BD(1)C4-C10	326.RY(1)C9	0.67	1.94	0.032
43.BD(1)C4-C10	328.RY(3)C9	0.61	1.80	0.030
44.BD(1)C5-C6	76.BD*(1)C1-C6	0.56	0.99	0.021
44.BD(1)C5-C6	78.BD*(1)C1-H11	3.17	0.84	0.046
44.BD(1)C5-C6	84.BD*(1)C4-C5	0.63	0.92	0.022
44.BD(1)C5-C6	86.BD*(1)C4-C10	2.67	0.94	0.045
44.BD(1)C5-C6	88.BD*(1)C5-C7	1.05	0.94	0.028
44.BD(1)C5-C6	89.BD*(1)C6-B14	0.85	0.84	0.024
44.BD(1)C5-C6	90.BD*(1)C7-C8	2.39	1.00	0.044
44.BD(1)C5-C6	118.RY(1)C1	0.76	1.80	0.033
44.BD(1)C5-C6	196.RY(1)C4	1.18	1.80	0.041
44.BD(1)C5-C6	274.RY(1)C7	0.69	1.86	0.032
45.BD(1)C5-C7	76.BD*(1)C1-C6	2.32	0.99	0.043
45.BD(1)C5-C7	82.BD*(1)C3-C4	2.76	0.94	0.045
45.BD(1)C5-C7	84.BD*(1)C4-C5	0.60	0.91	0.021
45.BD(1)C5-C7	87.BD*(1)C5-C6	1.01	0.94	0.027
45.BD(1)C5-C7	92.BD*(1)C7-B15	0.91	0.85	0.025
45.BD(1)C5-C7	94.BD*(1)C8-H16	3.20	0.85	0.046
45.BD(1)C5-C7	196.RY(1)C4	1.14	1.79	0.040
45.BD(1)C5-C7	248.RY(1)C6	0.62	1.83	0.030
45.BD(1)C5-C7	300.RY(1)C8	0.77	1.85	0.034
46.BD(1)C6-B14	75.BD*(1)C1-C2	5.16	0.83	0.058
46.BD(1)C6-B14	76.BD*(1)C1-C6	0.62	0.85	0.020
46.BD(1)C6-B14	78.BD*(1)C1-H11	0.70	0.71	0.020
46.BD(1)C6-B14	84.BD*(1)C4-C5	3.73	0.78	0.048
46.BD(1)C6-B14	87.BD*(1)C5-C6	0.52	0.81	0.018
46.BD(1)C6-B14	112.BD*(1)C21-H27	1.58	0.70	0.030
46.BD(1)C6-B14	116.BD*(1)C22-H31	1.59	0.70	0.030
46.BD(1)C6-B14	118.RY(1)C1	1.50	1.66	0.044
46.BD(1)C6-B14	222.RY(1)C5	1.06	1.68	0.038
46.BD(1)C6-B14	223.RY(2)C5	1.78	1.75	0.050
47.BD(1)C7-C8	87.BD*(1)C5-C6	3.59	0.96	0.052
47.BD(1)C7-C8	88.BD*(1)C5-C7	0.66	0.96	0.022
47.BD(1)C7-C8	92.BD*(1)C7-B15	1.51	0.87	0.032
47.BD(1)C7-C8	93.BD*(1)C8-C9	1.04	0.98	0.028
47.BD(1)C7-C8	94.BD*(1)C8-H16	0.50	0.87	0.019
47.BD(1)C7-C8	97.BD*(1)C9-H17	2.22	0.84	0.039
47.BD(1)C7-C8	104.BD*(1)B15-Se35	0.92	0.62	0.021
47.BD(1)C7-C8	222.RY(1)C5	1.25	1.83	0.043
47.BD(1)C7-C8	223.RY(2)C5	0.53	1.91	0.028
47.BD(1)C7-C8	326.RY(1)C9	0.61	1.93	0.031
47.BD(1)C7-C8	328.RY(3)C9	0.53	1.79	0.028
48.BD(2)C7-C8	85.BD*(2)C4-C5	12.48	0.22	0.047
48.BD(2)C7-C8	96.BD*(2)C9-C10	16.80	0.21	0.053

48.BD(2)C7-C8	102.BD*(1)B15-C19	2.95	0.54	0.036
48.BD(2)C7-C8	104.BD*(1)B15-Se35	3.71	0.33	0.031
48.BD(2)C7-C8	224.RY(3)C5	0.95	0.84	0.025
48.BD(2)C7-C8	327.RY(2)C9	1.54	0.72	0.030
49.BD(1)C7-B15	84.BD*(1)C4-C5	3.74	0.78	0.048
49.BD(1)C7-B15	88.BD*(1)C5-C7	0.52	0.80	0.018
49.BD(1)C7-B15	90.BD*(1)C7-C8	0.63	0.87	0.021
49.BD(1)C7-B15	93.BD*(1)C8-C9	4.81	0.83	0.056
49.BD(1)C7-B15	94.BD*(1)C8-H16	0.70	0.72	0.020
49.BD(1)C7-B15	106.BD*(1)C19-H24	1.76	0.70	0.031
49.BD(1)C7-B15	110.BD*(1)C20-H34	1.28	0.71	0.027
49.BD(1)C7-B15	222.RY(1)C5	1.46	1.68	0.044
49.BD(1)C7-B15	223.RY(2)C5	1.44	1.76	0.045
49.BD(1)C7-B15	300.RY(1)C8	1.71	1.72	0.048
50.BD(1)C8-C9	90.BD*(1)C7-C8	1.00	1.03	0.029
50.BD(1)C8-C9	92.BD*(1)C7-B15	2.28	0.88	0.040
50.BD(1)C8-C9	95.BD*(1)C9-C10	0.92	1.03	0.027
50.BD(1)C8-C9	98.BD*(1)C10-H18	2.91	0.85	0.044
50.BD(1)C8-C9	274.RY(1)C7	1.50	1.89	0.048
50.BD(1)C8-C9	352.RY(1)C10	0.72	1.99	0.034
51.BD(1)C8-H16	88.BD*(1)C5-C7	5.20	0.86	0.060
51.BD(1)C8-H16	95.BD*(1)C9-C10	3.66	0.92	0.052
51.BD(1)C8-H16	97.BD*(1)C9-H17	0.62	0.75	0.019
51.BD(1)C8-H16	110.BD*(1)C20-H34	0.64	0.76	0.020
51.BD(1)C8-H16	274.RY(1)C7	1.82	1.78	0.051
51.BD(1)C8-H16	326.RY(1)C9	1.06	1.84	0.039
52.BD(1)C9-C10	82.BD*(1)C3-C4	2.51	0.99	0.045
52.BD(1)C9-C10	86.BD*(1)C4-C10	0.90	0.99	0.027
52.BD(1)C9-C10	93.BD*(1)C8-C9	0.96	1.01	0.028
52.BD(1)C9-C10	94.BD*(1)C8-H16	2.02	0.90	0.038
52.BD(1)C9-C10	196.RY(1)C4	0.73	1.84	0.033
52.BD(1)C9-C10	197.RY(2)C4	0.83	2.10	0.037
52.BD(1)C9-C10	300.RY(1)C8	1.00	1.91	0.039
53.BD(2)C9-C10	85.BD*(2)C4-C5	13.64	0.24	0.051
53.BD(2)C9-C10	91.BD*(2)C7-C8	11.42	0.26	0.048
53.BD(2)C9-C10	198.RY(3)C4	0.58	0.77	0.019
53.BD(2)C9-C10	301.RY(2)C8	1.14	0.73	0.026
54.BD(1)C9-H17	86.BD*(1)C4-C10	4.07	0.88	0.054
54.BD(1)C9-H17	90.BD*(1)C7-C8	4.08	0.94	0.055
54.BD(1)C9-H17	94.BD*(1)C8-H16	0.53	0.80	0.018
54.BD(1)C9-H17	98.BD*(1)C10-H18	0.56	0.77	0.019
54.BD(1)C9-H17	300.RY(1)C8	1.13	1.80	0.040
54.BD(1)C9-H17	352.RY(1)C10	1.28	1.91	0.044
55.BD(1)C10-H18	84.BD*(1)C4-C5	4.72	0.86	0.057
55.BD(1)C10-H18	93.BD*(1)C8-C9	3.82	0.90	0.052
55.BD(1)C10-H18	97.BD*(1)C9-H17	0.57	0.77	0.019
55.BD(1)C10-H18	196.RY(1)C4	0.54	1.74	0.027
55.BD(1)C10-H18	197.RY(2)C4	1.10	1.99	0.042
55.BD(1)C10-H18	326.RY(1)C9	1.22	1.86	0.043
56.BD(1)B14-C21	77.BD*(2)C1-C6	2.22	0.38	0.026
56.BD(1)B14-C21	87.BD*(1)C5-C6	1.87	0.81	0.035
56.BD(1)B14-C21	111.BD*(1)C21-H26	0.54	0.71	0.017
56.BD(1)B14-C21	112.BD*(1)C21-H27	0.60	0.70	0.018
56.BD(1)B14-C21	113.BD*(1)C21-H28	0.55	0.70	0.018
56.BD(1)B14-C21	114.BD*(1)C22-H29	1.89	0.72	0.033
57.BD(1)B14-C22	77.BD*(2)C1-C6	1.63	0.38	0.022
57.BD(1)B14-C22	87.BD*(1)C5-C6	1.89	0.81	0.035
57.BD(1)B14-C22	111.BD*(1)C21-H26	1.84	0.71	0.032
57.BD(1)B14-C22	114.BD*(1)C22-H29	0.60	0.72	0.018
57.BD(1)B14-C22	115.BD*(1)C22-H30	0.57	0.70	0.018
57.BD(1)B14-C22	116.BD*(1)C22-H31	0.59	0.70	0.018
57.BD(1)B14-C22	117.BD*(1)Se35-H36	0.81	0.45	0.017
58.BD(1)B14-Se35	76.BD*(1)C1-C6	2.25	0.84	0.039
58.BD(1)B14-Se35	103.BD*(1)B15-C20	1.35	0.68	0.027
58.BD(1)B14-Se35	113.BD*(1)C21-H28	2.80	0.69	0.039
58.BD(1)B14-Se35	115.BD*(1)C22-H30	2.65	0.69	0.038
58.BD(1)B14-Se35	586.RY(1)C22	0.69	1.17	0.025
59.BD(1)B15-C19	90.BD*(1)C7-C8	0.80	0.86	0.023
59.BD(1)B15-C19	91.BD*(2)C7-C8	3.44	0.38	0.032
59.BD(1)B15-C19	105.BD*(1)C19-H23	0.61	0.72	0.019
59.BD(1)B15-C19	106.BD*(1)C19-H24	0.56	0.70	0.018
59.BD(1)B15-C19	107.BD*(1)C19-H25	0.54	0.70	0.017
59.BD(1)B15-C19	108.BD*(1)C20-H32	1.98	0.70	0.033

59.BD(1)B15-C19	117.BD*(1)Se35-H36	0.76	0.44	0.016
60.BD(1)B15-C20	88.BD*(1)C5-C7	3.02	0.81	0.044
60.BD(1)B15-C20	105.BD*(1)C19-H23	1.71	0.73	0.032
60.BD(1)B15-C20	108.BD*(1)C20-H32	0.56	0.71	0.018
60.BD(1)B15-C20	109.BD*(1)C20-H33	0.56	0.70	0.018
60.BD(1)B15-C20	110.BD*(1)C20-H34	0.68	0.71	0.020
61.BD(1)B15-Se35	89.BD*(1)C6-B14	0.61	0.68	0.018
61.BD(1)B15-Se35	90.BD*(1)C7-C8	1.92	0.84	0.036
61.BD(1)B15-Se35	91.BD*(2)C7-C8	1.57	0.36	0.021
61.BD(1)B15-Se35	99.BD*(1)B14-C21	1.02	0.66	0.023
61.BD(1)B15-Se35	107.BD*(1)C19-H25	2.40	0.68	0.036
61.BD(1)B15-Se35	109.BD*(1)C20-H33	2.90	0.67	0.039
61.BD(1)B15-Se35	508.RY(1)C19	0.66	1.18	0.025
62.BD(1)C19-H23	103.BD*(1)B15-C20	2.07	0.72	0.035
62.BD(1)C19-H23	444.RY(2)B15	0.78	1.46	0.030
63.BD(1)C19-H24	92.BD*(1)C7-B15	2.14	0.75	0.036
64.BD(1)C19-H25	102.BD*(1)B15-C19	0.84	0.71	0.022
64.BD(1)C19-H25	104.BD*(1)B15-Se35	3.99	0.50	0.040
65.BD(1)C20-H32	102.BD*(1)B15-C19	2.20	0.72	0.036
65.BD(1)C20-H32	444.RY(2)B15	0.78	1.47	0.030
66.BD(1)C20-H33	103.BD*(1)B15-C20	0.67	0.73	0.020
66.BD(1)C20-H33	104.BD*(1)B15-Se35	3.41	0.51	0.037
67.BD(1)C20-H34	92.BD*(1)C7-B15	2.71	0.75	0.040
67.BD(1)C20-H34	103.BD*(1)B15-C20	0.61	0.73	0.019
67.BD(1)C20-H34	443.RY(1)B15	0.68	1.47	0.028
68.BD(1)C21-H26	100.BD*(1)B14-C22	2.17	0.71	0.035
68.BD(1)C21-H26	418.RY(2)B14	0.69	1.42	0.028
69.BD(1)C21-H27	89.BD*(1)C6-B14	2.36	0.74	0.037
70.BD(1)C21-H28	99.BD*(1)B14-C21	0.71	0.72	0.020
70.BD(1)C21-H28	101.BD*(1)B14-Se35	3.20	0.51	0.036
71.BD(1)C22-H29	99.BD*(1)B14-C21	2.06	0.72	0.034
71.BD(1)C22-H29	418.RY(2)B14	1.02	1.42	0.034
72.BD(1)C22-H30	100.BD*(1)B14-C22	0.78	0.71	0.021
72.BD(1)C22-H30	101.BD*(1)B14-Se35	3.65	0.51	0.038
73.BD(1)C22-H31	89.BD*(1)C6-B14	2.52	0.74	0.038
73.BD(1)C22-H31	419.RY(3)B14	0.85	1.38	0.031
74.BD(1)Se35-H36	100.BD*(1)B14-C22	1.25	0.74	0.027
74.BD(1)Se35-H36	102.BD*(1)B15-C19	1.39	0.74	0.029

Table S26. Natural Bond Orbitals Summary for [**1**-SeH]$^-$ without Rydberg orbitals.

NBO	Occupancy	Energy / a.u.	Principal delocalizations (geminal,vicinal,remote)
1.CR(1)C1	1.99998	-9.74880	
2.CR(1)C2	1.99998	-9.76049	
3.CR(1)C3	1.99998	-9.75875	
4.CR(1)C4	1.99998	-9.76581	
5.CR(1)C5	1.99998	-9.76244	
6.CR(1)C6	1.99998	-9.73956	
7.CR(1)C7	1.99998	-9.73726	
8.CR(1)C8	1.99998	-9.74737	
9.CR(1)C9	1.99998	-9.76024	
10.CR(1)C10	1.99998	-9.75924	
11.CR(1)B14	1.99996	-6.33044	
12.CR(1)B15	1.99996	-6.32692	
13.CR(1)C19	1.99998	-9.71133	
14.CR(1)C20	1.99998	-9.71489	
15.CR(1)C21	1.99998	-9.71523	
16.CR(1)C22	1.99998	-9.71387	
17.CR(1)Se35	2.00000	-436.98892	
18.CR(2)Se35	2.00000	-65.78053	
19.CR(3)Se35	1.99998	-13.87252	
20.CR(4)Se35	2.00000	-21.34941	
21.CR(5)Se35	2.00000	-35.45954	
22.CR(6)Se35	2.00000	-21.35063	
23.CR(7)Se35	2.00000	-35.46023	
24.CR(8)Se35	2.00000	-21.35563	
25.CR(9)Se35	2.00000	-35.46298	
26.CR(10)Se35	1.99999	-1.82665	
27.CR(11)Se35	1.99998	-1.83111	
28.CR(12)Se35	1.99999	-1.83215	
29.CR(13)Se35	1.99999	-1.82653	
30.CR(14)Se35	1.99997	-1.83348	
31.LP(1)Se35	1.97750	-0.25486	89(v),92(v),417(v)
32.BD(1)C1-C2	1.98165	-0.39059	83(v),89(v),248(v),76(g)
			79(g),170(v)
33.BD(1)C1-C6	1.97021	-0.37593	88(v),81(v),101(v),89(g)
			75(g),222(v),223(v),87(g)
			144(v),146(v)
34.BD(2)C1-C6	1.67897	-0.08303	80(v),85(v),99(v),100(v)
			145(v),224(v),112(r)
35.BD(1)C1-H11	1.97195	-0.28427	87(v),79(v),248(v),144(v)
			101(r),81(v)
36.BD(1)C2-C3	1.98325	-0.40728	86(v),78(v),118(v),75(g)
			82(g),197(v),196(v)
37.BD(2)C2-C3	1.75548	-0.10639	85(v),77(v),119(v),198(v)
38.BD(1)C2-H12	1.97825	-0.30475	76(v),82(v),170(v),118(v)
			78(v),83(v)
39.BD(1)C3-C4	1.97613	-0.38610	81(v),88(v),95(v),222(v)
			352(v),79(g),84(g),86(g)
			144(v),146(v)
40.BD(1)C3-H13	1.97698	-0.30414	84(v),75(v),144(v),197(v)
			81(v),196(v)
41.BD(1)C4-C5	1.96764	-0.36383	89(v),92(v),83(v),98(v)
			248(v),274(v),82(g),87(g)
			86(g),88(g),172(v),354(v)
42.BD(2)C4-C5	1.52223	-0.07973	80(v),96(v),77(v),91(v)
			171(v),353(v),224(g)
43.BD(1)C4-C10	1.97594	-0.38516	97(v),87(v),79(v),222(v)
			170(v),95(g),84(g),82(g)
			326(v),328(v)
44.BD(1)C5-C6	1.97179	-0.36101	78(v),86(v),90(v),196(v)
			88(g),89(g),118(v),274(v)
			84(g),76(g)
45.BD(1)C5-C7	1.97135	-0.35669	94(v),82(v),76(v),196(v)
			87(g),92(g),300(v),248(v)
			84(g)
46.BD(1)C6-B14	1.94956	-0.22411	75(v),84(v),223(v),116(v)
			112(v),118(v),222(v),78(v)
			76(g),87(g)
47.BD(1)C7-C8	1.97298	-0.37765	87(v),97(v),92(g),222(v)
			93(g),104(v),88(g),326(v)

			328(v),223(v),94(g)
48.BD(2)C7-C8	1.69262	-0.08385	96(v),85(v),104(v),102(v)
			327(v),224(v)
49.BD(1)C7-B15	1.95082	-0.22592	93(v),84(v),106(v),300(v)
			222(v),223(v),110(v),94(v)
			90(g),88(g)
50.BD(1)C8-C9	1.98187	-0.38800	98(v),92(v),274(v),90(g)
			95(g),352(v)
51.BD(1)C8-H16	1.97273	-0.28269	88(v),95(v),274(v),326(v)
			110(r),97(v)
52.BD(1)C9-C10	1.98368	-0.40854	82(v),94(v),300(v),93(g)
			86(g),197(v),196(v)
53.BD(2)C9-C10	1.76638	-0.10717	85(v),91(v),301(v),198(v)
54.BD(1)C9-H17	1.97847	-0.30466	90(v),86(v),352(v),300(v)
			98(v),94(v)
55.BD(1)C10-H18	1.97698	-0.30422	84(v),93(v),326(v),197(v)
			97(v),196(v)
56.BD(1)B14-C21	1.96268	-0.22742	77(v),114(v),87(v),112(g)
			113(g),111(g)
57.BD(1)B14-C22	1.96512	-0.22887	87(v),111(v),77(v),117(v)
			114(g),116(g),115(g)
58.BD(1)B14-Se35	1.96151	-0.21184	113(v),115(v),76(v),103(v)
			586(v)
59.BD(1)B15-C19	1.95728	-0.22493	91(v),108(v),90(v),117(v)
			105(g),106(g),107(g)
60.BD(1)B15-C20	1.97659	-0.23056	88(v),105(v),110(g),108(g)
			109(g)
61.BD(1)B15-Se35	1.95259	-0.20549	109(v),107(v),90(v),91(v)
			99(v),508(v),89(v)
62.BD(1)C19-H23	1.98588	-0.25579	103(v),444(v)
63.BD(1)C19-H24	1.98482	-0.25773	92(v)
64.BD(1)C19-H25	1.97706	-0.25496	104(v),102(g)
65.BD(1)C20-H32	1.98790	-0.26190	102(v),444(v)
66.BD(1)C20-H33	1.97992	-0.26185	104(v),103(g)
67.BD(1)C20-H34	1.98582	-0.26023	92(v),443(v),103(g)
68.BD(1)C21-H26	1.98764	-0.25994	100(v),418(v)
69.BD(1)C21-H27	1.98478	-0.26032	89(v)
70.BD(1)C21-H28	1.97899	-0.26059	101(v),99(g)
71.BD(1)C22-H29	1.98680	-0.25936	99(v),418(v)
72.BD(1)C22-H30	1.97735	-0.25922	101(v),100(g)
73.BD(1)C22-H31	1.98595	-0.25873	89(v),419(v)
74.BD(1)Se35-H36	1.98591	-0.28251	102(v),100(v)
------non-Lewis---------			
75.BD*(1)C1-C2	0.02060	0.60576	
76.BD*(1)C1-C6	0.02028	0.62839	
77.BD*(2)C1-C6	0.26043	0.14994	
78.BD*(1)C1-H11	0.02079	0.48308	
79.BD*(1)C2-C3	0.01352	0.63592	
80.BD*(2)C2-C3	0.31293	0.12493	
81.BD*(1)C2-H12	0.01779	0.46349	
82.BD*(1)C3-C4	0.02039	0.58342	
83.BD*(1)C3-H13	0.01855	0.46234	
84.BD*(1)C4-C5	0.03859	0.55713	
85.BD*(2)C4-C5	0.46889	0.13642	
86.BD*(1)C4-C10	0.02059	0.57971	
87.BD*(1)C5-C6	0.03118	0.58307	
88.BD*(1)C5-C7	0.03056	0.57770	
89.BD*(1)C6-B14	0.03534	0.47682	
90.BD*(1)C7-C8	0.02065	0.63946	
91.BD*(2)C7-C8	0.25887	0.15064	
92.BD*(1)C7-B15	0.03274	0.48845	
93.BD*(1)C8-C9	0.02030	0.60000	
94.BD*(1)C8-H16	0.02036	0.49040	
95.BD*(1)C9-C10	0.01341	0.63883	
96.BD*(2)C9-C10	0.29980	0.12506	
97.BD*(1)C9-H17	0.01774	0.46377	
98.BD*(1)C10-H18	0.01860	0.46225	
99.BD*(1)B14-C21	0.02203	0.45596	
100.BD*(1)B14-C22	0.02238	0.45358	
101.BD*(1)B14-Se35	0.04850	0.24688	
102.BD*(1)B15-C19	0.02339	0.45693	
103.BD*(1)B15-C20	0.01885	0.46684	
104.BD*(1)B15-Se35	0.05974	0.24440	

105.BD*(1)C19-H23	0.00776	0.49918	
106.BD*(1)C19-H24	0.00859	0.47708	
107.BD*(1)C19-H25	0.00944	0.47533	
108.BD*(1)C20-H32	0.00815	0.47538	
109.BD*(1)C20-H33	0.01257	0.46878	
110.BD*(1)C20-H34	0.00775	0.48071	
111.BD*(1)C21-H26	0.00782	0.47807	
112.BD*(1)C21-H27	0.00847	0.47554	
113.BD*(1)C21-H28	0.01228	0.47338	
114.BD*(1)C22-H29	0.00838	0.49051	
115.BD*(1)C22-H30	0.01030	0.47321	
116.BD*(1)C22-H31	0.00865	0.47525	
117.BD*(1)Se35-H36	0.01982	0.21811	

Table S27. Second order perturbation analysis of the Fock matrix. In NBO-basis for [**1**-NH]$^{-}$. Threshold for printing the donor acceptor interactions in 0.50 kcal/mol. E(2) is the energy of the donor-acceptor interaction in kcal/mol, E(NL) – E(L) is the energy difference between the donor and acceptor in atomic units and F(L,NL) is the overlap between the donor and acceptor natural orbitals in atomic units.

Donor (L) NBO	Acceptor (NL) NBO	E(2) / kcal/mol	E(NL) – E(L) / a.u	F(L,NL) / a.u.
18.LP(1)C5	62.LV(1)C4	1181.32	0.01	0.107
18.LP(1)C5	65.BD*(2)C1-C6	79.96	0.12	0.087
18.LP(1)C5	68.BD*(2)C2-C3	1.75	0.09	0.011
18.LP(1)C5	78.BD*(2)C7-C8	79.96	0.12	0.087
18.LP(1)C5	83.BD*(2)C9-C10	1.75	0.09	0.011
18.LP(1)C5	186.RY(3)C4	1.68	0.62	0.029
18.LP(1)C5	191.RY(8)C4	1.07	2.79	0.049
18.LP(1)C5	212.RY(3)C5	3.43	0.70	0.044
18.LP(1)C5	238.RY(3)C6	1.06	0.73	0.025
18.LP(1)C5	241.RY(6)C6	0.77	2.72	0.041
18.LP(1)C5	264.RY(3)C7	1.06	0.73	0.025
18.LP(1)C5	267.RY(6)C7	0.77	2.72	0.041
19.BD(1)C1-C2	64.BD*(1)C1-C6	0.98	1.03	0.028
19.BD(1)C1-C2	67.BD*(1)C2-C3	0.90	1.02	0.027
19.BD(1)C1-C2	71.BD*(1)C3-H13	2.81	0.85	0.044
19.BD(1)C1-C2	76.BD*(1)C6-B14	1.97	0.90	0.038
19.BD(1)C1-C2	158.RY(1)C3	0.72	1.99	0.034
19.BD(1)C1-C2	236.RY(1)C6	1.58	2.07	0.051
20.BD(1)C1-C6	63.BD*(1)C1-C2	1.00	0.98	0.028
20.BD(1)C1-C6	69.BD*(1)C2-H12	2.28	0.84	0.039
20.BD(1)C1-C6	74.BD*(1)C5-C6	0.70	0.97	0.023
20.BD(1)C1-C6	75.BD*(1)C5-C7	3.49	0.97	0.052
20.BD(1)C1-C6	76.BD*(1)C6-B14	1.32	0.89	0.031
20.BD(1)C1-C6	88.BD*(1)B14-N35	0.59	0.80	0.019
20.BD(1)C1-C6	132.RY(1)C2	0.62	1.92	0.031
20.BD(1)C1-C6	134.RY(3)C2	0.53	1.79	0.028
20.BD(1)C1-C6	210.RY(1)C5	1.35	1.98	0.046
20.BD(1)C1-C6	211.RY(2)C5	0.62	2.07	0.032
20.BD(1)C1-C6	405.RY(1)B14	0.62	1.67	0.029
21.BD(2)C1-C6	68.BD*(2)C2-C3	17.73	0.21	0.054
21.BD(2)C1-C6	86.BD*(1)B14-C21	2.60	0.56	0.034
21.BD(2)C1-C6	87.BD*(1)B14-C22	1.19	0.55	0.023
21.BD(2)C1-C6	133.RY(2)C2	1.58	0.72	0.030
21.BD(2)C1-C6	212.RY(3)C5	0.75	0.82	0.022
22.BD(1)C1-H11	67.BD*(1)C2-C3	3.76	0.92	0.052
22.BD(1)C1-H11	69.BD*(1)C2-H12	0.61	0.75	0.019
22.BD(1)C1-H11	74.BD*(1)C5-C6	5.36	0.88	0.061
22.BD(1)C1-H11	132.RY(1)C2	1.07	1.82	0.039
22.BD(1)C1-H11	236.RY(1)C6	2.01	1.96	0.056
23.BD(1)C2-C3	63.BD*(1)C1-C2	0.95	1.01	0.028
23.BD(1)C2-C3	66.BD*(1)C1-H11	2.07	0.89	0.038
23.BD(1)C2-C3	70.BD*(1)C3-C4	0.92	0.99	0.027
23.BD(1)C2-C3	73.BD*(1)C4-C10	2.65	0.99	0.046
23.BD(1)C2-C3	106.RY(1)C1	1.00	1.94	0.039
23.BD(1)C2-C3	184.RY(1)C4	0.69	1.88	0.032
23.BD(1)C2-C3	185.RY(2)C4	0.80	2.11	0.037

24.BD(2)C2-C3	62.LV(1)C4	50.74	0.13	0.072
24.BD(2)C2-C3	65.BD*(2)C1-C6	10.94	0.26	0.048
24.BD(2)C2-C3	107.RY(2)C1	1.19	0.73	0.026
24.BD(2)C2-C3	186.RY(3)C4	0.65	0.76	0.020
25.BD(1)C2-H12	64.BD*(1)C1-C6	4.00	0.95	0.055
25.BD(1)C2-H12	66.BD*(1)C1-H11	0.55	0.79	0.019
25.BD(1)C2-H12	70.BD*(1)C3-C4	4.05	0.89	0.054
25.BD(1)C2-H12	71.BD*(1)C3-H13	0.57	0.77	0.019
25.BD(1)C2-H12	106.RY(1)C1	1.18	1.84	0.042
25.BD(1)C2-H12	158.RY(1)C3	1.28	1.91	0.044
26.BD(1)C3-C4	67.BD*(1)C2-C3	0.84	1.02	0.026
26.BD(1)C3-C4	69.BD*(1)C2-H12	2.75	0.85	0.043
26.BD(1)C3-C4	72.BD*(1)C4-C5	0.84	0.95	0.025
26.BD(1)C3-C4	73.BD*(1)C4-C10	0.73	0.97	0.024
26.BD(1)C3-C4	75.BD*(1)C5-C7	2.61	0.98	0.045
26.BD(1)C3-C4	82.BD*(1)C9-C10	1.95	1.02	0.040
26.BD(1)C3-C4	132.RY(1)C2	0.68	1.93	0.032
26.BD(1)C3-C4	134.RY(3)C2	0.57	1.80	0.029
26.BD(1)C3-C4	210.RY(1)C5	1.28	1.99	0.045
26.BD(1)C3-C4	340.RY(1)C10	0.97	1.99	0.039
27.BD(1)C3-H13	63.BD*(1)C1-C2	3.84	0.91	0.053
27.BD(1)C3-H13	69.BD*(1)C2-H12	0.57	0.77	0.019
27.BD(1)C3-H13	72.BD*(1)C4-C5	4.64	0.87	0.057
27.BD(1)C3-H13	132.RY(1)C2	1.21	1.84	0.042
27.BD(1)C3-H13	184.RY(1)C4	0.55	1.77	0.028
27.BD(1)C3-H13	185.RY(2)C4	1.09	2.01	0.042
28.BD(1)C4-C5	70.BD*(1)C3-C4	0.67	0.95	0.023
28.BD(1)C4-C5	71.BD*(1)C3-H13	2.44	0.82	0.040
28.BD(1)C4-C5	73.BD*(1)C4-C10	0.67	0.95	0.023
28.BD(1)C4-C5	74.BD*(1)C5-C6	0.65	0.96	0.022
28.BD(1)C4-C5	75.BD*(1)C5-C7	0.65	0.96	0.022
28.BD(1)C4-C5	76.BD*(1)C6-B14	2.15	0.87	0.039
28.BD(1)C4-C5	79.BD*(1)C7-B15	2.15	0.87	0.039
28.BD(1)C4-C5	85.BD*(1)C10-H18	2.44	0.82	0.040
28.BD(1)C4-C5	160.RY(3)C3	0.54	1.96	0.029
28.BD(1)C4-C5	236.RY(1)C6	0.74	2.04	0.035
28.BD(1)C4-C5	262.RY(1)C7	0.74	2.04	0.035
28.BD(1)C4-C5	342.RY(3)C10	0.54	1.96	0.029
29.BD(1)C4-C10	67.BD*(1)C2-C3	1.95	1.02	0.040
29.BD(1)C4-C10	70.BD*(1)C3-C4	0.73	0.97	0.024
29.BD(1)C4-C10	72.BD*(1)C4-C5	0.84	0.95	0.025
29.BD(1)C4-C10	74.BD*(1)C5-C6	2.61	0.98	0.045
29.BD(1)C4-C10	82.BD*(1)C9-C10	0.84	1.02	0.026
29.BD(1)C4-C10	84.BD*(1)C9-H17	2.75	0.85	0.043
29.BD(1)C4-C10	158.RY(1)C3	0.97	1.99	0.039
29.BD(1)C4-C10	210.RY(1)C5	1.28	1.99	0.045
29.BD(1)C4-C10	314.RY(1)C9	0.68	1.93	0.032
29.BD(1)C4-C10	316.RY(3)C9	0.57	1.80	0.029
30.BD(1)C5-C6	64.BD*(1)C1-C6	0.53	1.00	0.021
30.BD(1)C5-C6	66.BD*(1)C1-H11	3.27	0.84	0.047
30.BD(1)C5-C6	72.BD*(1)C4-C5	0.66	0.92	0.022
30.BD(1)C5-C6	73.BD*(1)C4-C10	2.67	0.94	0.045
30.BD(1)C5-C6	75.BD*(1)C5-C7	1.04	0.95	0.028
30.BD(1)C5-C6	76.BD*(1)C6-B14	0.75	0.87	0.023
30.BD(1)C5-C6	77.BD*(1)C7-C8	2.55	1.00	0.045
30.BD(1)C5-C6	106.RY(1)C1	0.75	1.89	0.034
30.BD(1)C5-C6	184.RY(1)C4	1.15	1.83	0.041
30.BD(1)C5-C6	262.RY(1)C7	0.70	2.04	0.034
31.BD(1)C5-C7	64.BD*(1)C1-C6	2.55	1.00	0.045
31.BD(1)C5-C7	70.BD*(1)C3-C4	2.67	0.94	0.045
31.BD(1)C5-C7	72.BD*(1)C4-C5	0.66	0.92	0.022
31.BD(1)C5-C7	74.BD*(1)C5-C6	1.04	0.95	0.028
31.BD(1)C5-C7	77.BD*(1)C7-C8	0.53	1.00	0.021
31.BD(1)C5-C7	79.BD*(1)C7-B15	0.75	0.87	0.023
31.BD(1)C5-C7	81.BD*(1)C8-H16	3.27	0.84	0.047
31.BD(1)C5-C7	184.RY(1)C4	1.15	1.83	0.041
31.BD(1)C5-C7	236.RY(1)C6	0.70	2.04	0.034
31.BD(1)C5-C7	288.RY(1)C8	0.75	1.89	0.034
32.BD(1)C6-B14	63.BD*(1)C1-C2	4.67	0.81	0.055
32.BD(1)C6-B14	64.BD*(1)C1-C6	0.56	0.85	0.020
32.BD(1)C6-B14	66.BD*(1)C1-H11	0.76	0.69	0.020
32.BD(1)C6-B14	72.BD*(1)C4-C5	4.11	0.77	0.050
32.BD(1)C6-B14	99.BD*(1)C21-H27	1.65	0.68	0.030

32.BD(1)C6-B14	103.BD*(1)C22-H31	1.45	0.68	0.028
32.BD(1)C6-B14	105.BD*(1)N35-H37	1.56	0.68	0.029
32.BD(1)C6-B14	106.RY(1)C1	2.16	1.74	0.055
32.BD(1)C6-B14	109.RY(4)C1	0.53	2.03	0.029
32.BD(1)C6-B14	210.RY(1)C5	1.69	1.81	0.049
32.BD(1)C6-B14	211.RY(2)C5	1.80	1.90	0.052
32.BD(1)C6-B14	236.RY(1)C6	0.59	1.89	0.030
32.BD(1)C6-B14	265.RY(4)C7	0.51	2.88	0.034
32.BD(1)C6-B14	414.RY(10)B14	0.54	2.68	0.034
32.BD(1)C6-B14	426.RY(22)B14	0.70	6.13	0.059
32.BD(1)C6-B14	428.RY(24)B14	0.67	5.10	0.052
33.BD(1)C7-C8	74.BD*(1)C5-C6	3.49	0.97	0.052
33.BD(1)C7-C8	75.BD*(1)C5-C7	0.70	0.97	0.023
33.BD(1)C7-C8	79.BD*(1)C7-B15	1.32	0.89	0.031
33.BD(1)C7-C8	80.BD*(1)C8-C9	1.00	0.98	0.028
33.BD(1)C7-C8	84.BD*(1)C9-H17	2.28	0.84	0.039
33.BD(1)C7-C8	91.BD*(1)B15-N35	0.59	0.80	0.019
33.BD(1)C7-C8	210.RY(1)C5	1.35	1.98	0.046
33.BD(1)C7-C8	211.RY(2)C5	0.62	2.07	0.032
33.BD(1)C7-C8	314.RY(1)C9	0.62	1.92	0.031
33.BD(1)C7-C8	316.RY(3)C9	0.53	1.79	0.028
33.BD(1)C7-C8	431.RY(1)B15	0.62	1.67	0.029
34.BD(2)C7-C8	83.BD*(2)C9-C10	17.73	0.21	0.054
34.BD(2)C7-C8	89.BD*(1)B15-C19	1.19	0.55	0.023
34.BD(2)C7-C8	90.BD*(1)B15-C20	2.60	0.56	0.034
34.BD(2)C7-C8	212.RY(3)C5	0.75	0.82	0.022
34.BD(2)C7-C8	315.RY(2)C9	1.58	0.72	0.030
35.BD(1)C7-B15	72.BD*(1)C4-C5	4.11	0.77	0.050
35.BD(1)C7-B15	77.BD*(1)C7-C8	0.56	0.85	0.020
35.BD(1)C7-B15	80.BD*(1)C8-C9	4.67	0.81	0.055
35.BD(1)C7-B15	81.BD*(1)C8-H16	0.76	0.69	0.020
35.BD(1)C7-B15	93.BD*(1)C19-H24	1.45	0.68	0.028
35.BD(1)C7-B15	97.BD*(1)C20-H34	1.65	0.68	0.030
35.BD(1)C7-B15	105.BD*(1)N35-H37	1.56	0.68	0.029
35.BD(1)C7-B15	210.RY(1)C5	1.69	1.81	0.049
35.BD(1)C7-B15	211.RY(2)C5	1.80	1.90	0.052
35.BD(1)C7-B15	239.RY(4)C6	0.51	2.88	0.034
35.BD(1)C7-B15	262.RY(1)C7	0.59	1.89	0.030
35.BD(1)C7-B15	288.RY(1)C8	2.16	1.74	0.055
35.BD(1)C7-B15	291.RY(4)C8	0.53	2.03	0.029
35.BD(1)C7-B15	440.RY(10)B15	0.54	2.68	0.034
35.BD(1)C7-B15	452.RY(22)B15	0.70	6.13	0.059
35.BD(1)C7-B15	454.RY(24)B15	0.67	5.10	0.052
36.BD(1)C8-C9	77.BD*(1)C7-C8	0.98	1.03	0.028
36.BD(1)C8-C9	79.BD*(1)C7-B15	1.97	0.90	0.038
36.BD(1)C8-C9	82.BD*(1)C9-C10	0.90	1.02	0.027
36.BD(1)C8-C9	85.BD*(1)C10-H18	2.81	0.85	0.044
36.BD(1)C8-C9	262.RY(1)C7	1.58	2.07	0.051
36.BD(1)C8-C9	340.RY(1)C10	0.72	1.99	0.034
37.BD(1)C8-H16	75.BD*(1)C5-C7	5.36	0.88	0.061
37.BD(1)C8-H16	82.BD*(1)C9-C10	3.76	0.92	0.052
37.BD(1)C8-H16	84.BD*(1)C9-H17	0.61	0.75	0.019
37.BD(1)C8-H16	262.RY(1)C7	2.01	1.96	0.056
37.BD(1)C8-H16	314.RY(1)C9	1.07	1.82	0.039
38.BD(1)C9-C10	70.BD*(1)C3-C4	2.65	0.99	0.046
38.BD(1)C9-C10	73.BD*(1)C4-C10	0.92	0.99	0.027
38.BD(1)C9-C10	80.BD*(1)C8-C9	0.95	1.01	0.028
38.BD(1)C9-C10	81.BD*(1)C8-H16	2.07	0.89	0.038
38.BD(1)C9-C10	184.RY(1)C4	0.69	1.88	0.032
38.BD(1)C9-C10	185.RY(2)C4	0.80	2.11	0.037
38.BD(1)C9-C10	288.RY(1)C8	1.00	1.94	0.039
39.BD(2)C9-C10	62.LV(1)C4	50.74	0.13	0.072
39.BD(2)C9-C10	78.BD*(2)C7-C8	10.94	0.26	0.048
39.BD(2)C9-C10	186.RY(3)C4	0.65	0.76	0.020
39.BD(2)C9-C10	289.RY(2)C8	1.19	0.73	0.026
40.BD(1)C9-H17	73.BD*(1)C4-C10	4.05	0.89	0.054
40.BD(1)C9-H17	77.BD*(1)C7-C8	4.00	0.95	0.055
40.BD(1)C9-H17	81.BD*(1)C8-H16	0.55	0.79	0.019
40.BD(1)C9-H17	85.BD*(1)C10-H18	0.57	0.77	0.019
40.BD(1)C9-H17	288.RY(1)C8	1.18	1.84	0.042
40.BD(1)C9-H17	340.RY(1)C10	1.28	1.91	0.044
41.BD(1)C10-H18	72.BD*(1)C4-C5	4.64	0.87	0.057
41.BD(1)C10-H18	80.BD*(1)C8-C9	3.84	0.91	0.053

41.BD(1)C10-H18	84.BD*(1)C9-H17	0.57	0.77	0.019
41.BD(1)C10-H18	184.RY(1)C4	0.55	1.77	0.028
41.BD(1)C10-H18	185.RY(2)C4	1.09	2.01	0.042
41.BD(1)C10-H18	314.RY(1)C9	1.21	1.84	0.042
42.BD(1)B14-C21	65.BD*(2)C1-C6	2.81	0.37	0.029
42.BD(1)B14-C21	74.BD*(1)C5-C6	0.88	0.80	0.024
42.BD(1)B14-C21	100.BD*(1)C21-H28	0.50	0.69	0.017
42.BD(1)B14-C21	101.BD*(1)C22-H29	1.82	0.68	0.031
42.BD(1)B14-C21	104.BD*(1)N35-H36	1.35	0.68	0.027
43.BD(1)B14-C22	65.BD*(2)C1-C6	1.11	0.37	0.018
43.BD(1)B14-C22	74.BD*(1)C5-C6	2.13	0.81	0.037
43.BD(1)B14-C22	91.BD*(1)B15-N35	1.41	0.64	0.027
43.BD(1)B14-C22	98.BD*(1)C21-H26	1.76	0.71	0.032
43.BD(1)B14-C22	102.BD*(1)C22-H30	0.51	0.69	0.017
44.BD(1)B14-N35	64.BD*(1)C1-C6	1.60	0.97	0.035
44.BD(1)B14-N35	89.BD*(1)B15-C19	0.63	0.80	0.020
44.BD(1)B14-N35	91.BD*(1)B15-N35	1.35	0.75	0.028
44.BD(1)B14-N35	100.BD*(1)C21-H28	1.02	0.81	0.026
44.BD(1)B14-N35	102.BD*(1)C22-H30	1.15	0.80	0.027
44.BD(1)B14-N35	104.BD*(1)N35-H36	0.62	0.79	0.020
44.BD(1)B14-N35	105.BD*(1)N35-H37	0.60	0.79	0.020
44.BD(1)B14-N35	433.RY(3)B15	0.75	2.16	0.036
45.BD(1)B15-C19	75.BD*(1)C5-C7	2.13	0.81	0.037
45.BD(1)B15-C19	78.BD*(2)C7-C8	1.11	0.37	0.018
45.BD(1)B15-C19	88.BD*(1)B14-N35	1.41	0.64	0.027
45.BD(1)B15-C19	94.BD*(1)C19-H25	0.51	0.69	0.017
45.BD(1)B15-C19	95.BD*(1)C20-H32	1.76	0.71	0.032
46.BD(1)B15-C20	75.BD*(1)C5-C7	0.88	0.80	0.024
46.BD(1)B15-C20	78.BD*(2)C7-C8	2.81	0.37	0.029
46.BD(1)B15-C20	92.BD*(1)C19-H23	1.82	0.68	0.031
46.BD(1)B15-C20	96.BD*(1)C20-H33	0.50	0.69	0.017
46.BD(1)B15-C20	104.BD*(1)N35-H36	1.35	0.68	0.027
47.BD(1)B15-N35	77.BD*(1)C7-C8	1.60	0.97	0.035
47.BD(1)B15-N35	87.BD*(1)B14-C22	0.63	0.80	0.020
47.BD(1)B15-N35	88.BD*(1)B14-N35	1.35	0.75	0.028
47.BD(1)B15-N35	94.BD*(1)C19-H25	1.15	0.80	0.027
47.BD(1)B15-N35	96.BD*(1)C20-H33	1.02	0.81	0.026
47.BD(1)B15-N35	104.BD*(1)N35-H36	0.62	0.79	0.020
47.BD(1)B15-N35	105.BD*(1)N35-H37	0.60	0.79	0.020
47.BD(1)B15-N35	407.RY(3)B14	0.75	2.16	0.036
48.BD(1)C19-H23	90.BD*(1)B15-C20	1.80	0.74	0.033
48.BD(1)C19-H23	433.RY(3)B15	0.66	2.10	0.033
49.BD(1)C19-H24	79.BD*(1)C7-B15	2.05	0.78	0.036
49.BD(1)C19-H24	435.RY(5)B15	0.99	1.72	0.037
50.BD(1)C19-H25	91.BD*(1)B15-N35	2.12	0.69	0.034
50.BD(1)C19-H25	433.RY(3)B15	0.79	2.10	0.036
51.BD(1)C20-H32	89.BD*(1)B15-C19	1.72	0.73	0.032
51.BD(1)C20-H32	433.RY(3)B15	0.67	2.09	0.033
52.BD(1)C20-H33	90.BD*(1)B15-C20	0.57	0.73	0.018
52.BD(1)C20-H33	91.BD*(1)B15-N35	2.70	0.68	0.038
52.BD(1)C20-H33	432.RY(2)B15	0.97	1.88	0.038
53.BD(1)C20-H34	79.BD*(1)C7-B15	1.97	0.77	0.035
53.BD(1)C20-H34	435.RY(5)B15	0.80	1.72	0.033
54.BD(1)C21-H26	87.BD*(1)B14-C22	1.72	0.73	0.032
54.BD(1)C21-H26	407.RY(3)B14	0.67	2.09	0.033
55.BD(1)C21-H27	76.BD*(1)C6-B14	1.97	0.77	0.035
55.BD(1)C21-H27	409.RY(5)B14	0.80	1.72	0.033
56.BD(1)C21-H28	86.BD*(1)B14-C21	0.57	0.73	0.018
56.BD(1)C21-H28	88.BD*(1)B14-N35	2.70	0.68	0.038
56.BD(1)C21-H28	406.RY(2)B14	0.97	1.88	0.038
57.BD(1)C22-H29	86.BD*(1)B14-C21	1.80	0.74	0.033
57.BD(1)C22-H29	407.RY(3)B14	0.66	2.10	0.033
58.BD(1)C22-H30	88.BD*(1)B14-N35	2.12	0.69	0.034
58.BD(1)C22-H30	407.RY(3)B14	0.79	2.10	0.036
59.BD(1)C22-H31	76.BD*(1)C6-B14	2.05	0.78	0.036
59.BD(1)C22-H31	409.RY(5)B14	0.99	1.72	0.037
60.BD(1)N35-H36	86.BD*(1)B14-C21	1.41	0.85	0.031
60.BD(1)N35-H36	88.BD*(1)B14-N35	0.74	0.80	0.022
60.BD(1)N35-H36	90.BD*(1)B15-C20	1.41	0.85	0.031
60.BD(1)N35-H36	91.BD*(1)B15-N35	0.74	0.80	0.022
60.BD(1)N35-H36	405.RY(1)B14	0.98	1.67	0.036
60.BD(1)N35-H36	406.RY(2)B14	0.72	2.00	0.034
60.BD(1)N35-H36	431.RY(1)B15	0.98	1.67	0.036

60.BD(1)N35-H36	432.RY(2)B15	0.72	2.00	0.034
60.BD(1)N35-H36	797.RY(3)H37	0.79	3.52	0.047
61.BD(1)N35-H37	76.BD*(1)C6-B14	1.21	0.89	0.029
61.BD(1)N35-H37	79.BD*(1)C7-B15	1.21	0.89	0.029
61.BD(1)N35-H37	88.BD*(1)B14-N35	0.68	0.81	0.021
61.BD(1)N35-H37	91.BD*(1)B15-N35	0.68	0.81	0.021
61.BD(1)N35-H37	405.RY(1)B14	0.64	1.68	0.029
61.BD(1)N35-H37	406.RY(2)B14	0.74	2.00	0.034
61.BD(1)N35-H37	431.RY(1)B15	0.64	1.68	0.029
61.BD(1)N35-H37	432.RY(2)B15	0.74	2.00	0.034
61.BD(1)N35-H37	784.RY(3)H36	0.73	3.60	0.046

Table S28. Natural Bond Orbitals Summary for [**1**-NH]$^{-}$ without Rydberg orbitals.

NBO	Occupancy	Energy / a.u.	Principal delocalizations (geminal,vicinal,remote)
1.CR(1)C1	1.99998	-9.74096	
2.CR(1)C2	1.99998	-9.75493	
3.CR(1)C3	1.99998	-9.75260	
4.CR(1)C4	1.99998	-9.75886	
5.CR(1)C5	1.99998	-9.75197	
6.CR(1)C6	1.99998	-9.72660	
7.CR(1)C7	1.99998	-9.72660	
8.CR(1)C8	1.99998	-9.74096	
9.CR(1)C9	1.99998	-9.75493	
10.CR(1)C10	1.99998	-9.75260	
11.CR(1)B14	1.99996	-6.30904	
12.CR(1)B15	1.99996	-6.30904	
13.CR(1)C19	1.99998	-9.70986	
14.CR(1)C20	1.99998	-9.70360	
15.CR(1)C21	1.99998	-9.70360	
16.CR(1)C22	1.99998	-9.70986	
17.CR(1)N35	1.99999	-13.85873	
18.LP(1)C5	1.00062	0.04073	62(v),65(v),78(v),212(g)
			68(r),83(r),186(v),191(v)
			238(v),264(v),241(v),267(v)
19.BD(1)C1-C2	1.98254	-0.38286	71(v),76(v),236(v),64(g)
			67(g),158(v)
20.BD(1)C1-C6	1.97566	-0.37065	75(v),69(v),210(v),76(g)
			63(g),74(g),405(v),211(v)
			132(v),88(v),134(v)
21.BD(2)C1-C6	1.67892	-0.07578	68(v),86(v),133(v),87(v)
			212(v)
22.BD(1)C1-H11	1.97466	-0.27766	74(v),67(v),236(v),132(v)
			69(v)
23.BD(1)C2-C3	1.98338	-0.40109	73(v),66(v),106(v),63(g)
			70(g),185(v),184(v)
24.BD(2)C2-C3	1.76238	-0.10036	62(v),65(v),107(v),186(v)
25.BD(1)C2-H12	1.97870	-0.29877	70(v),64(v),158(v),106(v)
			71(v),66(v)
26.BD(1)C3-C4	1.97662	-0.37964	69(v),75(v),82(v),210(v)
			340(v),67(g),72(g),73(g)
			132(v),134(v)
27.BD(1)C3-H13	1.97742	-0.29807	72(v),63(v),132(v),185(v)
			69(v),184(v)
28.BD(1)C4-C5	1.96912	-0.35732	71(v),85(v),76(v),79(v)
			236(v),262(v),70(g),73(g)
			74(g),75(g),160(v),342(v)
29.BD(1)C4-C10	1.97662	-0.37964	84(v),74(v),67(v),210(v)
			158(v),82(g),72(g),70(g)
			314(v),316(v)
30.BD(1)C5-C6	1.97080	-0.35063	66(v),73(v),77(v),184(v)
			75(g),76(g),106(v),262(v)
			72(g),64(g)
31.BD(1)C5-C7	1.97080	-0.35063	81(v),70(v),64(v),184(v)
			74(g),79(g),288(v),236(v)
			72(g),77(g)
32.BD(1)C6-B14	1.94427	-0.20487	63(v),72(v),106(v),211(v)
			210(v),99(v),105(v),103(v)
			66(v),426(g),428(g),236(g)

			64(g),414(g),109(v),265(r)
33.BD(1)C7-C8	1.97566	-0.37065	74(v),84(v),210(v),79(g)
			80(g),75(g),431(v),211(v)
			314(v),91(v),316(v)
34.BD(2)C7-C8	1.67892	-0.07578	83(v),90(v),315(v),89(v)
			212(v)
35.BD(1)C7-B15	1.94427	-0.20487	80(v),72(v),288(v),211(v)
			210(v),97(v),105(v),93(v)
			81(v),452(g),454(g),262(g)
			77(g),440(g),291(v),239(r)
36.BD(1)C8-C9	1.98254	-0.38286	85(v),79(v),262(v),77(g)
			82(g),340(v)
37.BD(1)C8-H16	1.97466	-0.27766	75(v),82(v),262(v),314(v)
			84(v)
38.BD(1)C9-C10	1.98338	-0.40109	70(v),81(v),288(v),80(g)
			73(g),185(v),184(v)
39.BD(2)C9-C10	1.76238	-0.10036	62(v),78(v),289(v),186(v)
40.BD(1)C9-H17	1.97870	-0.29877	73(v),77(v),340(v),288(v)
			85(v),81(v)
41.BD(1)C10-H18	1.97742	-0.29807	72(v),80(v),314(v),185(v)
			84(v),184(v)
42.BD(1)B14-C21	1.95965	-0.20573	65(v),101(v),104(v),74(v)
			100(g)
43.BD(1)B14-C22	1.96928	-0.20862	74(v),98(v),91(v),65(v)
			102(g)
44.BD(1)B14-N35	1.97833	-0.32130	64(v),91(g),102(v),100(v)
			433(v),89(v),104(g),105(g)
45.BD(1)B15-C19	1.96928	-0.20862	75(v),95(v),88(v),78(v)
			94(g)
46.BD(1)B15-C20	1.95965	-0.20573	78(v),92(v),104(v),75(v)
			96(g)
47.BD(1)B15-N35	1.97833	-0.32130	77(v),88(g),94(v),96(v)
			407(v),87(v),104(g),105(g)
48.BD(1)C19-H23	1.98905	-0.25918	90(v),433(v)
49.BD(1)C19-H24	1.98716	-0.25925	79(v),435(v)
50.BD(1)C19-H25	1.98649	-0.25975	91(v),433(v)
51.BD(1)C20-H32	1.98790	-0.25107	89(v),433(v)
52.BD(1)C20-H33	1.98447	-0.25069	91(v),432(v),90(g)
53.BD(1)C20-H34	1.98582	-0.25338	79(v),435(v)
54.BD(1)C21-H26	1.98790	-0.25107	87(v),407(v)
55.BD(1)C21-H27	1.98582	-0.25338	76(v),409(v)
56.BD(1)C21-H28	1.98447	-0.25069	88(v),406(v),86(g)
57.BD(1)C22-H29	1.98905	-0.25918	86(v),407(v)
58.BD(1)C22-H30	1.98649	-0.25975	88(v),407(v)
59.BD(1)C22-H31	1.98716	-0.25925	76(v),409(v)
60.BD(1)N35-H36	1.98276	-0.37241	86(v),90(v),405(v),431(v)
			797(v),88(g),91(g),406(v)
			432(v)
61.BD(1)N35-H37	1.98462	-0.37662	76(v),79(v),406(v),432(v)
			784(v),88(g),91(g),405(v)
			431(v)
------non-LewiS--------- -------------------------			
62.LV(1)C4	0.99681	0.02847	
63.BD*(1)C1-C2	0.01955	0.60739	
64.BD*(1)C1-C6	0.01803	0.64944	
65.BD*(2)C1-C6	0.25512	0.15998	
66.BD*(1)C1-H11	0.02052	0.48964	
67.BD*(1)C2-C3	0.01340	0.63975	
68.BD*(2)C2-C3	0.31277	0.13034	
69.BD*(1)C2-H12	0.01751	0.46896	
70.BD*(1)C3-C4	0.02063	0.58934	
71.BD*(1)C3-H13	0.01869	0.46716	
72.BD*(1)C4-C5	0.03903	0.56739	
73.BD*(1)C4-C10	0.02063	0.58934	
74.BD*(1)C5-C6	0.02915	0.59788	
75.BD*(1)C5-C7	0.02915	0.59788	
76.BD*(1)C6-B14	0.02840	0.51603	
77.BD*(1)C7-C8	0.01803	0.64944	
78.BD*(2)C7-C8	0.25512	0.15998	
79.BD*(1)C7-B15	0.02840	0.51603	
80.BD*(1)C8-C9	0.01955	0.60739	
81.BD*(1)C8-H16	0.02052	0.48964	

82.BD*(1)C9-C10	0.01340	0.63975	
83.BD*(2)C9-C10	0.31277	0.13034	
84.BD*(1)C9-H17	0.01751	0.46896	
85.BD*(1)C10-H18	0.01869	0.46716	
86.BD*(1)B14-C21	0.02115	0.48068	
87.BD*(1)B14-C22	0.01776	0.47734	
88.BD*(1)B14-N35	0.03314	0.43135	
89.BD*(1)B15-C19	0.01776	0.47734	
90.BD*(1)B15-C20	0.02115	0.48068	
91.BD*(1)B15-N35	0.03314	0.43135	
92.BD*(1)C19-H23	0.00746	0.47548	
93.BD*(1)C19-H24	0.00790	0.47148	
94.BD*(1)C19-H25	0.00615	0.48156	
95.BD*(1)C20-H32	0.00779	0.50229	
96.BD*(1)C20-H33	0.00512	0.48612	
97.BD*(1)C20-H34	0.00842	0.47484	
98.BD*(1)C21-H26	0.00779	0.50229	
99.BD*(1)C21-H27	0.00842	0.47484	
100.BD*(1)C21-H28	0.00512	0.48612	
101.BD*(1)C22-H29	0.00746	0.47548	
102.BD*(1)C22-H30	0.00615	0.48156	
103.BD*(1)C22-H31	0.00790	0.47148	
104.BD*(1)N35-H36	0.01664	0.47131	
105.BD*(1)N35-H37	0.01759	0.47171	

Table S29. Second order perturbation analysis of the Fock matrix. In NBO-basis for [**1**-PH]$^{-}$. Threshold for printing the donor acceptor interactions in 0.50 kcal/mol. E(2) is the energy of the donor-acceptor interaction in kcal/mol, E(NL) – E(L) is the energy difference between the donor and acceptor in atomic units and F(L,NL) is the overlap between the donor and acceptor natural orbitals in atomic units.

Donor (L) NBO		Acceptor (NL) NBO	E(2) / kcal/mol	E(NL) – E(L) / a.u	F(L,NL) / a.u.
22.BD(1)C1-C2		67.BD*(1)C1-C6	1.04	1.03	0.029
22.BD(1)C1-C2		70.BD*(1)C2-C3	0.92	1.03	0.027
22.BD(1)C1-C2		74.BD*(1)C3-H13	2.90	0.85	0.044
22.BD(1)C1-C2		80.BD*(1)C6-B14	2.16	0.87	0.039
22.BD(1)C1-C2		162.RY(1)C3	0.72	1.99	0.034
22.BD(1)C1-C2		240.RY(1)C6	1.49	1.86	0.047
23.BD(1)C1-C6		66.BD*(1)C1-C2	1.07	0.98	0.029
23.BD(1)C1-C6		69.BD*(1)C1-H11	0.54	0.87	0.019
23.BD(1)C1-C6		72.BD*(1)C2-H12	2.21	0.84	0.039
23.BD(1)C1-C6		78.BD*(1)C5-C6	0.64	0.95	0.022
23.BD(1)C1-C6		79.BD*(1)C5-C7	3.66	0.96	0.053
23.BD(1)C1-C6		80.BD*(1)C6-B14	1.36	0.86	0.031
23.BD(1)C1-C6		92.BD*(1)B14-P35	0.58	0.70	0.018
23.BD(1)C1-C6		136.RY(1)C2	0.62	1.93	0.031
23.BD(1)C1-C6		138.RY(3)C2	0.52	1.81	0.027
23.BD(1)C1-C6		214.RY(1)C5	1.30	1.89	0.044
23.BD(1)C1-C6		215.RY(2)C5	0.51	1.86	0.028
24.BD(2)C1-C6		71.BD*(2)C2-C3	16.85	0.21	0.053
24.BD(2)C1-C6		76.BD*(2)C4-C5	12.47	0.22	0.047
24.BD(2)C1-C6		91.BD*(1)B14-C22	3.05	0.54	0.036
24.BD(2)C1-C6		92.BD*(1)B14-P35	1.88	0.40	0.025
24.BD(2)C1-C6		137.RY(2)C2	1.56	0.72	0.030
24.BD(2)C1-C6		216.RY(3)C5	1.00	0.83	0.026
25.BD(1)C1-H11		70.BD*(1)C2-C3	3.66	0.92	0.052
25.BD(1)C1-H11		72.BD*(1)C2-H12	0.62	0.75	0.019
25.BD(1)C1-H11		78.BD*(1)C5-C6	5.38	0.86	0.061
25.BD(1)C1-H11		103.BD*(1)C21-H27	0.63	0.76	0.020
25.BD(1)C1-H11		136.RY(1)C2	1.06	1.83	0.039
25.BD(1)C1-H11		240.RY(1)C6	1.68	1.75	0.048
25.BD(1)C1-H11		241.RY(2)C6	0.77	1.75	0.033
26.BD(1)C2-C3		66.BD*(1)C1-C2	0.97	1.01	0.028
26.BD(1)C2-C3		69.BD*(1)C1-H11	2.03	0.90	0.038
26.BD(1)C2-C3		73.BD*(1)C3-C4	0.90	0.99	0.027
26.BD(1)C2-C3		77.BD*(1)C4-C10	2.50	0.99	0.044
26.BD(1)C2-C3		110.RY(1)C1	1.02	1.91	0.039
26.BD(1)C2-C3		188.RY(1)C4	0.73	1.84	0.033
26.BD(1)C2-C3		189.RY(2)C4	0.80	2.08	0.036
27.BD(2)C2-C3		68.BD*(2)C1-C6	11.41	0.26	0.048
27.BD(2)C2-C3		76.BD*(2)C4-C5	13.80	0.24	0.052
27.BD(2)C2-C3		111.RY(2)C1	1.11	0.75	0.026
27.BD(2)C2-C3		190.RY(3)C4	0.53	0.80	0.018
28.BD(1)C2-H12		67.BD*(1)C1-C6	4.12	0.95	0.056
28.BD(1)C2-H12		69.BD*(1)C1-H11	0.53	0.80	0.018
28.BD(1)C2-H12		73.BD*(1)C3-C4	4.06	0.89	0.054
28.BD(1)C2-H12		74.BD*(1)C3-H13	0.56	0.77	0.019
28.BD(1)C2-H12		110.RY(1)C1	1.15	1.81	0.041
28.BD(1)C2-H12		162.RY(1)C3	1.26	1.91	0.044
29.BD(1)C3-C4		70.BD*(1)C2-C3	0.85	1.02	0.026
29.BD(1)C3-C4		72.BD*(1)C2-H12	2.82	0.85	0.044
29.BD(1)C3-C4		75.BD*(1)C4-C5	0.81	0.94	0.025
29.BD(1)C3-C4		77.BD*(1)C4-C10	0.70	0.97	0.023
29.BD(1)C3-C4		79.BD*(1)C5-C7	2.61	0.97	0.045
29.BD(1)C3-C4		86.BD*(1)C9-C10	2.04	1.02	0.041
29.BD(1)C3-C4		136.RY(1)C2	0.67	1.94	0.032
29.BD(1)C3-C4		138.RY(3)C2	0.61	1.81	0.030
29.BD(1)C3-C4		214.RY(1)C5	1.22	1.89	0.043
29.BD(1)C3-C4		344.RY(1)C10	1.00	1.99	0.040
30.BD(1)C3-H13		66.BD*(1)C1-C2	3.81	0.91	0.052
30.BD(1)C3-H13		72.BD*(1)C2-H12	0.57	0.77	0.019
30.BD(1)C3-H13		75.BD*(1)C4-C5	4.73	0.86	0.057
30.BD(1)C3-H13		136.RY(1)C2	1.22	1.86	0.042
30.BD(1)C3-H13		188.RY(1)C4	0.55	1.74	0.028
30.BD(1)C3-H13		189.RY(2)C4	1.06	1.97	0.041

31.BD(1)C4-C5		73.BD*(1)C3-C4	0.66	0.94	0.022
31.BD(1)C4-C5		74.BD*(1)C3-H13	2.34	0.83	0.039
31.BD(1)C4-C5		77.BD*(1)C4-C10	0.68	0.95	0.023
31.BD(1)C4-C5		78.BD*(1)C5-C6	0.60	0.94	0.021
31.BD(1)C4-C5		79.BD*(1)C5-C7	0.65	0.94	0.022
31.BD(1)C4-C5		80.BD*(1)C6-B14	2.45	0.84	0.041
31.BD(1)C4-C5		83.BD*(1)C7-B15	2.61	0.84	0.042
31.BD(1)C4-C5		89.BD*(1)C10-H18	2.36	0.83	0.039
31.BD(1)C4-C5		164.RY(3)C3	0.53	1.87	0.028
31.BD(1)C4-C5		240.RY(1)C6	0.92	1.83	0.037
31.BD(1)C4-C5		266.RY(1)C7	0.79	1.90	0.035
31.BD(1)C4-C5		346.RY(3)C10	0.55	1.91	0.029
32.BD(2)C4-C5		68.BD*(2)C1-C6	14.70	0.23	0.052
32.BD(2)C4-C5		71.BD*(2)C2-C3	15.15	0.20	0.050
32.BD(2)C4-C5		82.BD*(2)C7-C8	14.95	0.23	0.053
32.BD(2)C4-C5		87.BD*(2)C9-C10	15.22	0.20	0.050
32.BD(2)C4-C5		163.RY(2)C3	0.95	0.76	0.024
32.BD(2)C4-C5		216.RY(3)C5	0.52	0.82	0.018
32.BD(2)C4-C5		242.RY(3)C6	0.58	0.92	0.021
32.BD(2)C4-C5		268.RY(3)C7	0.57	0.80	0.019
32.BD(2)C4-C5		345.RY(2)C10	1.00	0.74	0.024
33.BD(1)C4-C10		70.BD*(1)C2-C3	2.03	1.02	0.041
33.BD(1)C4-C10		73.BD*(1)C3-C4	0.71	0.97	0.023
33.BD(1)C4-C10		75.BD*(1)C4-C5	0.83	0.94	0.025
33.BD(1)C4-C10		78.BD*(1)C5-C6	2.56	0.96	0.044
33.BD(1)C4-C10		86.BD*(1)C9-C10	0.86	1.02	0.027
33.BD(1)C4-C10		88.BD*(1)C9-H17	2.80	0.85	0.044
33.BD(1)C4-C10		162.RY(1)C3	0.99	1.99	0.040
33.BD(1)C4-C10		214.RY(1)C5	1.19	1.89	0.042
33.BD(1)C4-C10		318.RY(1)C9	0.68	1.93	0.032
33.BD(1)C4-C10		320.RY(3)C9	0.60	1.83	0.029
34.BD(1)C5-C6		69.BD*(1)C1-H11	3.21	0.85	0.047
34.BD(1)C5-C6		75.BD*(1)C4-C5	0.60	0.91	0.021
34.BD(1)C5-C6		77.BD*(1)C4-C10	2.75	0.94	0.045
34.BD(1)C5-C6		79.BD*(1)C5-C7	1.00	0.94	0.027
34.BD(1)C5-C6		80.BD*(1)C6-B14	0.69	0.84	0.021
34.BD(1)C5-C6		81.BD*(1)C7-C8	2.34	0.99	0.043
34.BD(1)C5-C6		110.RY(1)C1	0.76	1.86	0.034
34.BD(1)C5-C6		188.RY(1)C4	1.14	1.79	0.040
34.BD(1)C5-C6		266.RY(1)C7	0.60	1.89	0.030
35.BD(1)C5-C7		67.BD*(1)C1-C6	2.42	1.00	0.044
35.BD(1)C5-C7		73.BD*(1)C3-C4	2.70	0.94	0.045
35.BD(1)C5-C7		75.BD*(1)C4-C5	0.63	0.92	0.021
35.BD(1)C5-C7		78.BD*(1)C5-C6	1.03	0.93	0.028
35.BD(1)C5-C7		81.BD*(1)C7-C8	0.54	0.99	0.021
35.BD(1)C5-C7		83.BD*(1)C7-B15	0.63	0.84	0.021
35.BD(1)C5-C7		85.BD*(1)C8-H16	3.17	0.84	0.046
35.BD(1)C5-C7		188.RY(1)C4	1.17	1.80	0.041
35.BD(1)C5-C7		240.RY(1)C6	0.80	1.83	0.034
35.BD(1)C5-C7		292.RY(1)C8	0.75	1.81	0.033
36.BD(1)C6-B14		66.BD*(1)C1-C2	4.91	0.82	0.057
36.BD(1)C6-B14		69.BD*(1)C1-H11	0.81	0.71	0.021
36.BD(1)C6-B14		75.BD*(1)C4-C5	3.69	0.77	0.048
36.BD(1)C6-B14		103.BD*(1)C21-H27	1.20	0.70	0.026
36.BD(1)C6-B14		107.BD*(1)C22-H31	1.68	0.69	0.031
36.BD(1)C6-B14		109.BD*(1)P35-H37	2.42	0.51	0.031
36.BD(1)C6-B14		110.RY(1)C1	1.76	1.72	0.049
36.BD(1)C6-B14		214.RY(1)C5	1.45	1.72	0.045
36.BD(1)C6-B14		215.RY(2)C5	1.45	1.70	0.044
37.BD(1)C7-C8		78.BD*(1)C5-C6	3.74	0.95	0.053
37.BD(1)C7-C8		79.BD*(1)C5-C7	0.65	0.96	0.022
37.BD(1)C7-C8		83.BD*(1)C7-B15	1.38	0.85	0.031
37.BD(1)C7-C8		84.BD*(1)C8-C9	1.05	0.98	0.029
37.BD(1)C7-C8		88.BD*(1)C9-H17	2.27	0.84	0.039
37.BD(1)C7-C8		95.BD*(1)B15-P35	1.06	0.70	0.024
37.BD(1)C7-C8		214.RY(1)C5	1.19	1.89	0.042
37.BD(1)C7-C8		215.RY(2)C5	0.69	1.86	0.032
37.BD(1)C7-C8		318.RY(1)C9	0.63	1.92	0.031
37.BD(1)C7-C8		320.RY(3)C9	0.59	1.82	0.029
38.BD(2)C7-C8		76.BD*(2)C4-C5	12.98	0.22	0.048
38.BD(2)C7-C8		87.BD*(2)C9-C10	17.30	0.21	0.053
38.BD(2)C7-C8		93.BD*(1)B15-C19	2.29	0.54	0.031
38.BD(2)C7-C8		94.BD*(1)B15-C20	1.95	0.54	0.029

38.BD(2)C7-C8		216.RY(3)C5	0.68	0.83	0.021
38.BD(2)C7-C8		319.RY(2)C9	1.63	0.72	0.030
39.BD(1)C7-B15		75.BD*(1)C4-C5	3.74	0.77	0.048
39.BD(1)C7-B15		84.BD*(1)C8-C9	5.18	0.82	0.058
39.BD(1)C7-B15		85.BD*(1)C8-H16	0.80	0.70	0.021
39.BD(1)C7-B15		97.BD*(1)C19-H24	1.51	0.69	0.029
39.BD(1)C7-B15		101.BD*(1)C20-H34	1.42	0.69	0.028
39.BD(1)C7-B15		109.BD*(1)P35-H37	1.54	0.51	0.025
39.BD(1)C7-B15		214.RY(1)C5	1.38	1.72	0.044
39.BD(1)C7-B15		215.RY(2)C5	1.63	1.70	0.047
39.BD(1)C7-B15		292.RY(1)C8	1.62	1.66	0.046
40.BD(1)C8-C9		81.BD*(1)C7-C8	1.03	1.02	0.029
40.BD(1)C8-C9		83.BD*(1)C7-B15	2.11	0.87	0.038
40.BD(1)C8-C9		86.BD*(1)C9-C10	0.94	1.03	0.028
40.BD(1)C8-C9		89.BD*(1)C10-H18	2.86	0.85	0.044
40.BD(1)C8-C9		266.RY(1)C7	1.47	1.92	0.048
40.BD(1)C8-C9		344.RY(1)C10	0.70	2.00	0.033
41.BD(1)C8-H16		79.BD*(1)C5-C7	5.39	0.86	0.061
41.BD(1)C8-H16		86.BD*(1)C9-C10	3.70	0.92	0.052
41.BD(1)C8-H16		88.BD*(1)C9-H17	0.64	0.75	0.019
41.BD(1)C8-H16		95.BD*(1)B15-P35	0.63	0.60	0.017
41.BD(1)C8-H16		266.RY(1)C7	2.00	1.82	0.054
41.BD(1)C8-H16		318.RY(1)C9	1.07	1.83	0.040
42.BD(1)C9-C10		73.BD*(1)C3-C4	2.53	0.99	0.045
42.BD(1)C9-C10		77.BD*(1)C4-C10	0.90	0.99	0.027
42.BD(1)C9-C10		84.BD*(1)C8-C9	1.01	1.01	0.029
42.BD(1)C9-C10		85.BD*(1)C8-H16	2.10	0.89	0.039
42.BD(1)C9-C10		188.RY(1)C4	0.66	1.84	0.031
42.BD(1)C9-C10		189.RY(2)C4	0.86	2.08	0.038
42.BD(1)C9-C10		292.RY(1)C8	1.06	1.85	0.040
43.BD(2)C9-C10		76.BD*(2)C4-C5	14.04	0.24	0.052
43.BD(2)C9-C10		82.BD*(2)C7-C8	11.56	0.26	0.049
43.BD(2)C9-C10		190.RY(3)C4	0.50	0.80	0.018
43.BD(2)C9-C10		293.RY(2)C8	1.03	0.74	0.025
44.BD(1)C9-H17		77.BD*(1)C4-C10	3.99	0.89	0.053
44.BD(1)C9-H17		81.BD*(1)C7-C8	4.16	0.94	0.056
44.BD(1)C9-H17		85.BD*(1)C8-H16	0.55	0.79	0.019
44.BD(1)C9-H17		89.BD*(1)C10-H18	0.55	0.77	0.018
44.BD(1)C9-H17		292.RY(1)C8	1.11	1.75	0.039
44.BD(1)C9-H17		344.RY(1)C10	1.25	1.91	0.044
45.BD(1)C10-H18		75.BD*(1)C4-C5	4.75	0.86	0.057
45.BD(1)C10-H18		84.BD*(1)C8-C9	3.77	0.91	0.052
45.BD(1)C10-H18		88.BD*(1)C9-H17	0.57	0.77	0.019
45.BD(1)C10-H18		188.RY(1)C4	0.50	1.74	0.026
45.BD(1)C10-H18		189.RY(2)C4	1.10	1.97	0.042
45.BD(1)C10-H18		318.RY(1)C9	1.20	1.85	0.042
46.BD(1)B14-C21		78.BD*(1)C5-C6	2.77	0.80	0.042
46.BD(1)B14-C21		80.BD*(1)C6-B14	0.61	0.70	0.019
46.BD(1)B14-C21		95.BD*(1)B15-P35	0.61	0.54	0.016
46.BD(1)B14-C21		103.BD*(1)C21-H27	0.55	0.70	0.018
46.BD(1)B14-C21		105.BD*(1)C22-H29	1.56	0.72	0.030
47.BD(1)B14-C22		67.BD*(1)C1-C6	0.54	0.86	0.019
47.BD(1)B14-C22		68.BD*(2)C1-C6	3.74	0.37	0.033
47.BD(1)B14-C22		80.BD*(1)C6-B14	0.56	0.70	0.018
47.BD(1)B14-C22		102.BD*(1)C21-H26	1.81	0.69	0.032
47.BD(1)B14-C22		108.BD*(1)P35-H36	1.70	0.51	0.026
48.BD(1)B14-P35		67.BD*(1)C1-C6	2.51	0.86	0.041
48.BD(1)B14-P35		68.BD*(2)C1-C6	1.40	0.37	0.020
48.BD(1)B14-P35		94.BD*(1)B15-C20	0.97	0.68	0.023
48.BD(1)B14-P35		104.BD*(1)C21-H28	2.48	0.69	0.037
48.BD(1)B14-P35		106.BD*(1)C22-H30	2.19	0.70	0.035
48.BD(1)B14-P35		108.BD*(1)P35-H36	0.76	0.51	0.018
48.BD(1)B14-P35		109.BD*(1)P35-H37	0.86	0.51	0.019
48.BD(1)B14-P35		241.RY(2)C6	0.71	1.69	0.031
48.BD(1)B14-P35		578.RY(1)C22	0.68	1.32	0.027
49.BD(1)B15-C19		79.BD*(1)C5-C7	1.70	0.80	0.033
49.BD(1)B15-C19		82.BD*(2)C7-C8	1.81	0.37	0.023
49.BD(1)B15-C19		99.BD*(1)C20-H32	1.72	0.70	0.031
49.BD(1)B15-C19		108.BD*(1)P35-H36	1.43	0.51	0.024
49.BD(1)B15-C19		762.RY(3)P35	0.58	1.45	0.026
50.BD(1)B15-C20		79.BD*(1)C5-C7	1.97	0.80	0.035
50.BD(1)B15-C20		82.BD*(2)C7-C8	1.72	0.37	0.023
50.BD(1)B15-C20		83.BD*(1)C7-B15	0.56	0.70	0.018

50.BD(1)B15-C20		92.BD*(1)B14-P35	0.56	0.54	0.015
50.BD(1)B15-C20		96.BD*(1)C19-H23	1.77	0.71	0.032
51.BD(1)B15-P35		81.BD*(1)C7-C8	2.81	0.85	0.044
51.BD(1)B15-P35		90.BD*(1)B14-C21	1.28	0.68	0.026
51.BD(1)B15-P35		98.BD*(1)C19-H25	2.33	0.69	0.036
51.BD(1)B15-P35		100.BD*(1)C20-H33	2.42	0.69	0.037
51.BD(1)B15-P35		108.BD*(1)P35-H36	0.79	0.51	0.018
51.BD(1)B15-P35		109.BD*(1)P35-H37	0.86	0.51	0.019
51.BD(1)B15-P35		267.RY(2)C7	0.75	1.48	0.030
51.BD(1)B15-P35		411.RY(3)B14	0.50	1.96	0.028
51.BD(1)B15-P35		500.RY(1)C19	0.71	1.37	0.028
51.BD(1)B15-P35		526.RY(1)C20	0.56	1.34	0.024
52.BD(1)C19-H23		94.BD*(1)B15-C20	1.84	0.72	0.033
52.BD(1)C19-H23		435.RY(1)B15	1.11	1.50	0.036
53.BD(1)C19-H24		83.BD*(1)C7-B15	2.31	0.74	0.037
54.BD(1)C19-H25		93.BD*(1)B15-C19	0.80	0.71	0.021
54.BD(1)C19-H25		95.BD*(1)B15-P35	2.59	0.58	0.035
54.BD(1)C19-H25		439.RY(5)B15	0.60	1.96	0.031
55.BD(1)C20-H32		93.BD*(1)B15-C19	2.00	0.72	0.034
55.BD(1)C20-H32		435.RY(1)B15	1.13	1.50	0.037
56.BD(1)C20-H33		94.BD*(1)B15-C20	0.67	0.72	0.020
56.BD(1)C20-H33		95.BD*(1)B15-P35	2.33	0.58	0.033
56.BD(1)C20-H33		437.RY(3)B15	0.51	1.95	0.028
57.BD(1)C20-H34		83.BD*(1)C7-B15	2.31	0.74	0.037
57.BD(1)C20-H34		438.RY(4)B15	0.77	1.59	0.031
58.BD(1)C21-H26		91.BD*(1)B14-C22	2.07	0.72	0.034
58.BD(1)C21-H26		409.RY(1)B14	0.81	1.52	0.031
58.BD(1)C21-H26		410.RY(2)B14	0.52	1.72	0.027
59.BD(1)C21-H27		80.BD*(1)C6-B14	2.70	0.74	0.040
59.BD(1)C21-H27		90.BD*(1)B14-C21	0.58	0.73	0.018
59.BD(1)C21-H27		411.RY(3)B14	0.66	2.00	0.032
60.BD(1)C21-H28		90.BD*(1)B14-C21	0.64	0.73	0.019
60.BD(1)C21-H28		92.BD*(1)B14-P35	2.46	0.58	0.034
60.BD(1)C21-H28		411.RY(3)B14	0.54	2.00	0.029
61.BD(1)C22-H29		90.BD*(1)B14-C21	1.85	0.72	0.033
61.BD(1)C22-H29		409.RY(1)B14	0.65	1.51	0.028
61.BD(1)C22-H29		410.RY(2)B14	0.60	1.71	0.029
62.BD(1)C22-H30		91.BD*(1)B14-C22	0.84	0.71	0.022
62.BD(1)C22-H30		92.BD*(1)B14-P35	2.76	0.57	0.036
63.BD(1)C22-H31		80.BD*(1)C6-B14	2.02	0.74	0.034
63.BD(1)C22-H31		412.RY(4)B14	0.72	1.82	0.032
64.BD(1)P35-H36		91.BD*(1)B14-C22	1.17	0.72	0.026
64.BD(1)P35-H36		92.BD*(1)B14-P35	0.81	0.59	0.019
64.BD(1)P35-H36		93.BD*(1)B15-C19	0.87	0.73	0.022
64.BD(1)P35-H36		95.BD*(1)B15-P35	0.93	0.59	0.021
64.BD(1)P35-H36		109.BD*(1)P35-H37	1.34	0.56	0.025
65.BD(1)P35-H37		80.BD*(1)C6-B14	0.78	0.75	0.022
65.BD(1)P35-H37		83.BD*(1)C7-B15	0.81	0.75	0.022
65.BD(1)P35-H37		92.BD*(1)B14-P35	1.09	0.59	0.023
65.BD(1)P35-H37		95.BD*(1)B15-P35	0.93	0.59	0.021
65.BD(1)P35-H37		108.BD*(1)P35-H36	1.28	0.57	0.024
65.BD(1)P35-H37		413.RY(5)B14	0.55	1.77	0.028

Table S30. Natural Bond Orbitals Summary for [**1**-PH]$^-$ without Rydberg orbitals.

NBO	Occupancy	Energy / a.u.	Principal delocalizations (geminal,vicinal,remote)
1.CR(1)C1	1.99998	-9.74571	
2.CR(1)C2	1.99998	-9.75887	
3.CR(1)C3	1.99998	-9.75768	
4.CR(1)C4	1.99998	-9.76446	
5.CR(1)C5	1.99998	-9.76181	
6.CR(1)C6	1.99998	-9.73918	
7.CR(1)C7	1.99998	-9.73895	
8.CR(1)C8	1.99998	-9.74622	
9.CR(1)C9	1.99998	-9.75880	

10.CR(1)C10	1.99998	-9.75714	
11.CR(1)B14	1.99996	-6.31104	
12.CR(1)B15	1.99996	-6.31234	
13.CR(1)C19	1.99998	-9.71350	
14.CR(1)C20	1.99998	-9.71379	
15.CR(1)C21	1.99998	-9.71469	
16.CR(1)C22	1.99998	-9.71183	
17.CR(1)P35	2.00000	-71.81482	
18.CR(2)P35	1.99997	-10.50134	
19.CR(3)P35	1.99998	-4.37354	
20.CR(4)P35	1.99999	-4.37781	
21.CR(5)P35	1.99999	-4.37770	
22.BD(1)C1-C2	1.98141	-0.38659	74(v),80(v),240(v),67(g)
			70(g),162(v)
23.BD(1)C1-C6	1.97442	-0.37774	79(v),72(v),80(g),214(v)
			66(g),78(g),136(v),92(v)
			69(g),138(v),215(v)
24.BD(2)C1-C6	1.69241	-0.08269	71(v),76(v),91(v),92(v)
			137(v),216(v)
25.BD(1)C1-H11	1.97281	-0.28058	78(v),70(v),240(v),136(v)
			241(v),103(r),72(v)
26.BD(1)C2-C3	1.98366	-0.40704	77(v),69(v),110(v),66(g)
			73(g),189(v),188(v)
27.BD(2)C2-C3	1.76457	-0.10566	76(v),68(v),111(v),190(v)
28.BD(1)C2-H12	1.97846	-0.30328	67(v),73(v),162(v),110(v)
			74(v),69(v)
29.BD(1)C3-C4	1.97606	-0.38379	72(v),79(v),86(v),214(v)
			344(v),70(g),75(g),77(g)
			136(v),138(v)
30.BD(1)C3-H13	1.97700	-0.30275	75(v),66(v),136(v),189(v)
			72(v),188(v)
31.BD(1)C4-C5	1.96728	-0.36199	83(v),80(v),89(v),74(v)
			240(v),266(v),77(g),73(g)
			79(g),78(g),346(v),164(v)
32.BD(2)C4-C5	1.52163	-0.07837	87(v),71(v),82(v),68(v)
			345(v),163(v),242(v),268(v)
			216(g)
33.BD(1)C4-C10	1.97612	-0.38439	88(v),78(v),70(v),214(v)
			162(v),86(g),75(g),73(g)
			318(v),320(v)
34.BD(1)C5-C6	1.97251	-0.35655	69(v),77(v),81(v),188(v)
			79(g),110(v),80(g),266(v)
			75(g)
35.BD(1)C5-C7	1.97297	-0.35908	85(v),73(v),67(v),188(v)
			78(g),240(v),292(v),83(g)
			75(g),81(g)
36.BD(1)C6-B14	1.93259	-0.21490	66(v),75(v),109(v),110(v)
			107(v),214(v),215(v),103(v)
			69(v)
37.BD(1)C7-C8	1.97320	-0.37535	78(v),88(v),83(g),214(v)
			95(v),84(g),215(v),79(g)
			318(v),320(v)
38.BD(2)C7-C8	1.67887	-0.08108	87(v),76(v),93(v),94(v)
			319(v),216(v)
39.BD(1)C7-B15	1.93785	-0.21330	84(v),75(v),215(v),292(v)
			109(v),97(v),101(v),214(v)
			85(v)
40.BD(1)C8-C9	1.98157	-0.38845	89(v),83(v),266(v),81(g)
			86(g),344(v)
41.BD(1)C8-H16	1.97291	-0.28140	79(v),86(v),266(v),318(v)
			88(v),95(r)
42.BD(1)C9-C10	1.98329	-0.40577	73(v),85(v),292(v),84(g)
			77(g),189(v),188(v)
43.BD(2)C9-C10	1.75624	-0.10487	76(v),82(v),293(v),190(v)
44.BD(1)C9-H17	1.97840	-0.30315	81(v),77(v),344(v),292(v)
			89(v),85(v)
45.BD(1)C10-H18	1.97701	-0.30254	75(v),84(v),318(v),189(v)
			88(v),188(v)
46.BD(1)B14-C21	1.97449	-0.22236	78(v),105(v),80(g),95(v)
			103(g)
47.BD(1)B14-C22	1.94751	-0.21453	68(v),102(v),108(v),80(g)
			67(v)
48.BD(1)B14-P35	1.95528	-0.21587	67(v),104(v),106(v),68(v)

			94(v),109(g),108(g),241(v)
			578(v)
49.BD(1)B15-C19	1.95794	-0.21786	82(v),99(v),79(v),108(v)
			762(v)
50.BD(1)B15-C20	1.96302	-0.21780	79(v),96(v),82(v),83(g)
			92(v)
51.BD(1)B15-P35	1.96246	-0.21603	81(v),100(v),98(v),90(v)
			109(g),108(g),267(v),500(v)
			526(v),411(v)
52.BD(1)C19-H23	1.98835	-0.25841	94(v),435(v)
53.BD(1)C19-H24	1.98684	-0.25817	83(v)
54.BD(1)C19-H25	1.98159	-0.25711	95(v),93(g),439(v)
55.BD(1)C20-H32	1.98916	-0.25811	93(v),435(v)
56.BD(1)C20-H33	1.98379	-0.25886	95(v),94(g),437(v)
57.BD(1)C20-H34	1.98585	-0.25894	83(v),438(v)
58.BD(1)C21-H26	1.98890	-0.26088	91(v),409(v),410(v)
59.BD(1)C21-H27	1.98655	-0.26010	80(v),411(v),90(g)
60.BD(1)C21-H28	1.98436	-0.26073	92(v),90(g),411(v)
61.BD(1)C22-H29	1.98770	-0.25578	90(v),409(v),410(v)
62.BD(1)C22-H30	1.98184	-0.25387	92(v),91(g)
63.BD(1)C22-H31	1.98626	-0.25730	80(v),412(v)
64.BD(1)P35-H36	1.98454	-0.26772	109(g),91(v),95(g),93(v)
			92(g)
65.BD(1)P35-H37	1.98429	-0.27095	108(g),92(g),95(g),83(v)
			80(v),413(v)
------non-LewiS-------- ----------			
66.BD*(1)C1-C2	0.02024	0.60257	
67.BD*(1)C1-C6	0.02019	0.64328	
68.BD*(2)C1-C6	0.25759	0.15244	
69.BD*(1)C1-H11	0.02079	0.49192	
70.BD*(1)C2-C3	0.01345	0.64029	
71.BD*(2)C2-C3	0.30177	0.12643	
72.BD*(1)C2-H12	0.01778	0.46504	
73.BD*(1)C3-C4	0.02057	0.58181	
74.BD*(1)C3-H13	0.01866	0.46345	
75.BD*(1)C4-C5	0.03929	0.55662	
76.BD*(2)C4-C5	0.47252	0.13721	
77.BD*(1)C4-C10	0.02039	0.58459	
78.BD*(1)C5-C6	0.02993	0.57575	
79.BD*(1)C5-C7	0.03058	0.58192	
80.BD*(1)C6-B14	0.03020	0.48109	
81.BD*(1)C7-C8	0.01995	0.63554	
82.BD*(2)C7-C8	0.25693	0.15318	
83.BD*(1)C7-B15	0.03045	0.47841	
84.BD*(1)C8-C9	0.02021	0.60788	
85.BD*(1)C8-H16	0.02123	0.48556	
86.BD*(1)C9-C10	0.01354	0.63800	
87.BD*(2)C9-C10	0.31207	0.12655	
88.BD*(1)C9-H17	0.01788	0.46495	
89.BD*(1)C10-H18	0.01860	0.46360	
90.BD*(1)B14-C21	0.01733	0.46893	
91.BD*(1)B14-C22	0.02220	0.45691	
92.BD*(1)B14-P35	0.03896	0.32037	
93.BD*(1)B15-C19	0.01985	0.45783	
94.BD*(1)B15-C20	0.01994	0.46056	
95.BD*(1)B15-P35	0.03522	0.32039	
96.BD*(1)C19-H23	0.00763	0.49561	
97.BD*(1)C19-H24	0.00808	0.47747	
98.BD*(1)C19-H25	0.00979	0.47860	
99.BD*(1)C20-H32	0.00690	0.48417	
100.BD*(1)C20-H33	0.01115	0.47856	
101.BD*(1)C20-H34	0.00752	0.47737	
102.BD*(1)C21-H26	0.00724	0.48022	
103.BD*(1)C21-H27	0.00710	0.48107	
104.BD*(1)C21-H28	0.01156	0.47351	
105.BD*(1)C22-H29	0.00684	0.50101	
106.BD*(1)C22-H30	0.00936	0.48118	
107.BD*(1)C22-H31	0.00790	0.48009	
108.BD*(1)P35-H36	0.03604	0.29627	
109.BD*(1)P35-H37	0.04214	0.29559	

Table S31. Second order perturbation analysis of the Fock matrix. In NBO-basis for [**1**-AsH]⁻. Threshold for printing the donor acceptor interactions in 0.50 kcal/mol. E(2) is the energy of the donor-acceptor interaction in kcal/mol, E(NL) – E(L) is the energy difference between the donor and acceptor in atomic units and F(L,NL) is the overlap between the donor and acceptor natural orbitals in atomic units.

Donor (L) NBO	Acceptor (NL) NBO	E(2) / kcal/mol	E(NL) – E(L) / a.u	F(L,NL) / a.u.
31.BD(1)C1-C2	76.BD*(1)C1-C6	1.03	1.03	0.029
31.BD(1)C1-C2	79.BD*(1)C2-C3	0.93	1.03	0.028
31.BD(1)C1-C2	83.BD*(1)C3-H13	2.92	0.85	0.045
31.BD(1)C1-C2	89.BD*(1)C6-B14	2.22	0.87	0.039
31.BD(1)C1-C2	171.RY(1)C3	0.72	1.99	0.034
31.BD(1)C1-C2	249.RY(1)C6	1.51	1.80	0.046
31.BD(1)C1-C2	254.RY(6)C6	0.50	3.30	0.036
32.BD(1)C1-C6	75.BD*(1)C1-C2	1.07	0.98	0.029
32.BD(1)C1-C6	78.BD*(1)C1-H11	0.53	0.87	0.019
32.BD(1)C1-C6	81.BD*(1)C2-H12	2.21	0.84	0.039
32.BD(1)C1-C6	87.BD*(1)C5-C6	0.65	0.95	0.022
32.BD(1)C1-C6	88.BD*(1)C5-C7	3.67	0.96	0.053
32.BD(1)C1-C6	89.BD*(1)C6-B14	1.42	0.86	0.031
32.BD(1)C1-C6	101.BD*(1)B14-As35	0.68	0.65	0.019
32.BD(1)C1-C6	145.RY(1)C2	0.61	1.93	0.031
32.BD(1)C1-C6	147.RY(3)C2	0.54	1.81	0.028
32.BD(1)C1-C6	223.RY(1)C5	1.24	1.84	0.043
32.BD(1)C1-C6	224.RY(2)C5	0.50	1.84	0.027
32.BD(1)C1-C6	418.RY(1)B14	0.56	1.61	0.027
33.BD(2)C1-C6	80.BD*(2)C2-C3	16.66	0.21	0.053
33.BD(2)C1-C6	85.BD*(2)C4-C5	12.22	0.22	0.046
33.BD(2)C1-C6	100.BD*(1)B14-C22	2.97	0.54	0.036
33.BD(2)C1-C6	101.BD*(1)B14-As35	2.58	0.36	0.027
33.BD(2)C1-C6	146.RY(2)C2	1.55	0.72	0.030
33.BD(2)C1-C6	225.RY(3)C5	0.97	0.84	0.025
34.BD(1)C1-H11	79.BD*(1)C2-C3	3.65	0.92	0.052
34.BD(1)C1-H11	81.BD*(1)C2-H12	0.62	0.75	0.019
34.BD(1)C1-H11	87.BD*(1)C5-C6	5.29	0.85	0.060
34.BD(1)C1-H11	112.BD*(1)C21-H27	0.70	0.76	0.021
34.BD(1)C1-H11	145.RY(1)C2	1.06	1.84	0.039
34.BD(1)C1-H11	249.RY(1)C6	1.62	1.69	0.047
34.BD(1)C1-H11	250.RY(2)C6	0.80	1.60	0.032
35.BD(1)C2-C3	75.BD*(1)C1-C2	0.97	1.01	0.028
35.BD(1)C2-C3	78.BD*(1)C1-H11	2.02	0.90	0.038
35.BD(1)C2-C3	82.BD*(1)C3-C4	0.90	0.99	0.027
35.BD(1)C2-C3	86.BD*(1)C4-C10	2.47	0.99	0.044
35.BD(1)C2-C3	119.RY(1)C1	1.02	1.89	0.039
35.BD(1)C2-C3	197.RY(1)C4	0.72	1.83	0.032
35.BD(1)C2-C3	198.RY(2)C4	0.84	2.08	0.037
36.BD(2)C2-C3	77.BD*(2)C1-C6	11.60	0.26	0.049
36.BD(2)C2-C3	85.BD*(2)C4-C5	13.77	0.24	0.052
36.BD(2)C2-C3	120.RY(2)C1	1.08	0.75	0.026
36.BD(2)C2-C3	199.RY(3)C4	0.54	0.79	0.018
37.BD(1)C2-H12	76.BD*(1)C1-C6	4.13	0.94	0.056
37.BD(1)C2-H12	78.BD*(1)C1-H11	0.53	0.80	0.018
37.BD(1)C2-H12	82.BD*(1)C3-C4	4.06	0.88	0.053
37.BD(1)C2-H12	83.BD*(1)C3-H13	0.56	0.77	0.018
37.BD(1)C2-H12	119.RY(1)C1	1.12	1.79	0.040
37.BD(1)C2-H12	171.RY(1)C3	1.26	1.91	0.044
38.BD(1)C3-C4	79.BD*(1)C2-C3	0.86	1.02	0.026
38.BD(1)C3-C4	81.BD*(1)C2-H12	2.83	0.85	0.044
38.BD(1)C3-C4	84.BD*(1)C4-C5	0.81	0.94	0.025
38.BD(1)C3-C4	86.BD*(1)C4-C10	0.70	0.97	0.023
38.BD(1)C3-C4	88.BD*(1)C5-C7	2.60	0.96	0.045
38.BD(1)C3-C4	95.BD*(1)C9-C10	2.06	1.02	0.041
38.BD(1)C3-C4	145.RY(1)C2	0.67	1.94	0.032
38.BD(1)C3-C4	147.RY(3)C2	0.61	1.81	0.030
38.BD(1)C3-C4	223.RY(1)C5	1.21	1.84	0.042
38.BD(1)C3-C4	353.RY(1)C10	1.00	1.99	0.040
39.BD(1)C3-H13	75.BD*(1)C1-C2	3.80	0.91	0.052
39.BD(1)C3-H13	81.BD*(1)C2-H12	0.57	0.77	0.019

39.BD(1)C3-H13	84.BD*(1)C4-C5	4.76	0.86	0.057
39.BD(1)C3-H13	145.RY(1)C2	1.22	1.86	0.042
39.BD(1)C3-H13	197.RY(1)C4	0.52	1.73	0.027
39.BD(1)C3-H13	198.RY(2)C4	1.09	1.98	0.041
40.BD(1)C4-C5	82.BD*(1)C3-C4	0.65	0.94	0.022
40.BD(1)C4-C5	83.BD*(1)C3-H13	2.31	0.83	0.039
40.BD(1)C4-C5	86.BD*(1)C4-C10	0.67	0.95	0.023
40.BD(1)C4-C5	87.BD*(1)C5-C6	0.58	0.93	0.021
40.BD(1)C4-C5	88.BD*(1)C5-C7	0.64	0.94	0.022
40.BD(1)C4-C5	89.BD*(1)C6-B14	2.54	0.84	0.041
40.BD(1)C4-C5	92.BD*(1)C7-B15	2.74	0.84	0.043
40.BD(1)C4-C5	98.BD*(1)C10-H18	2.34	0.83	0.039
40.BD(1)C4-C5	173.RY(3)C3	0.52	1.84	0.028
40.BD(1)C4-C5	249.RY(1)C6	0.91	1.77	0.036
40.BD(1)C4-C5	275.RY(1)C7	0.83	1.84	0.035
40.BD(1)C4-C5	355.RY(3)C10	0.55	1.88	0.029
41.BD(2)C4-C5	77.BD*(2)C1-C6	14.45	0.23	0.051
41.BD(2)C4-C5	80.BD*(2)C2-C3	15.17	0.21	0.050
41.BD(2)C4-C5	91.BD*(2)C7-C8	14.78	0.23	0.052
41.BD(2)C4-C5	96.BD*(2)C9-C10	15.24	0.21	0.050
41.BD(2)C4-C5	172.RY(2)C3	0.89	0.79	0.024
41.BD(2)C4-C5	225.RY(3)C5	0.52	0.84	0.019
41.BD(2)C4-C5	277.RY(3)C7	0.55	0.80	0.019
41.BD(2)C4-C5	354.RY(2)C10	0.94	0.76	0.024
42.BD(1)C4-C10	79.BD*(1)C2-C3	2.05	1.03	0.041
42.BD(1)C4-C10	82.BD*(1)C3-C4	0.70	0.97	0.023
42.BD(1)C4-C10	84.BD*(1)C4-C5	0.82	0.94	0.025
42.BD(1)C4-C10	87.BD*(1)C5-C6	2.53	0.96	0.044
42.BD(1)C4-C10	95.BD*(1)C9-C10	0.87	1.02	0.027
42.BD(1)C4-C10	97.BD*(1)C9-H17	2.81	0.85	0.044
42.BD(1)C4-C10	171.RY(1)C3	1.00	1.99	0.040
42.BD(1)C4-C10	223.RY(1)C5	1.16	1.84	0.041
42.BD(1)C4-C10	327.RY(1)C9	0.68	1.93	0.032
42.BD(1)C4-C10	329.RY(3)C9	0.60	1.83	0.030
43.BD(1)C5-C6	78.BD*(1)C1-H11	3.19	0.85	0.046
43.BD(1)C5-C6	84.BD*(1)C4-C5	0.58	0.91	0.020
43.BD(1)C5-C6	86.BD*(1)C4-C10	2.77	0.94	0.046
43.BD(1)C5-C6	88.BD*(1)C5-C7	0.97	0.93	0.027
43.BD(1)C5-C6	89.BD*(1)C6-B14	0.78	0.84	0.023
43.BD(1)C5-C6	90.BD*(1)C7-C8	2.27	0.99	0.042
43.BD(1)C5-C6	119.RY(1)C1	0.77	1.84	0.034
43.BD(1)C5-C6	197.RY(1)C4	1.13	1.78	0.040
43.BD(1)C5-C6	275.RY(1)C7	0.59	1.83	0.029
44.BD(1)C5-C7	76.BD*(1)C1-C6	2.34	1.00	0.043
44.BD(1)C5-C7	82.BD*(1)C3-C4	2.71	0.94	0.045
44.BD(1)C5-C7	84.BD*(1)C4-C5	0.62	0.91	0.021
44.BD(1)C5-C7	87.BD*(1)C5-C6	1.01	0.93	0.027
44.BD(1)C5-C7	90.BD*(1)C7-C8	0.54	0.99	0.021
44.BD(1)C5-C7	92.BD*(1)C7-B15	0.70	0.83	0.021
44.BD(1)C5-C7	94.BD*(1)C8-H16	3.15	0.85	0.046
44.BD(1)C5-C7	197.RY(1)C4	1.17	1.78	0.041
44.BD(1)C5-C7	249.RY(1)C6	0.73	1.77	0.032
44.BD(1)C5-C7	301.RY(1)C8	0.75	1.79	0.033
45.BD(1)C6-B14	75.BD*(1)C1-C2	4.96	0.82	0.057
45.BD(1)C6-B14	78.BD*(1)C1-H11	0.78	0.71	0.021
45.BD(1)C6-B14	84.BD*(1)C4-C5	3.57	0.77	0.047
45.BD(1)C6-B14	112.BD*(1)C21-H27	1.20	0.70	0.026
45.BD(1)C6-B14	116.BD*(1)C22-H31	1.72	0.70	0.031
45.BD(1)C6-B14	118.BD*(1)As35-H37	2.46	0.47	0.030
45.BD(1)C6-B14	119.RY(1)C1	1.68	1.70	0.048
45.BD(1)C6-B14	223.RY(1)C5	1.39	1.68	0.043
45.BD(1)C6-B14	224.RY(2)C5	1.35	1.68	0.042
46.BD(1)C7-C8	87.BD*(1)C5-C6	3.77	0.95	0.053
46.BD(1)C7-C8	88.BD*(1)C5-C7	0.65	0.95	0.022
46.BD(1)C7-C8	92.BD*(1)C7-B15	1.43	0.85	0.031
46.BD(1)C7-C8	93.BD*(1)C8-C9	1.06	0.98	0.029
46.BD(1)C7-C8	97.BD*(1)C9-H17	2.27	0.84	0.039
46.BD(1)C7-C8	104.BD*(1)B15-As35	1.42	0.65	0.027
46.BD(1)C7-C8	223.RY(1)C5	1.06	1.83	0.039
46.BD(1)C7-C8	224.RY(2)C5	0.74	1.83	0.033
46.BD(1)C7-C8	327.RY(1)C9	0.63	1.92	0.031
46.BD(1)C7-C8	329.RY(3)C9	0.61	1.82	0.030
47.BD(2)C7-C8	85.BD*(2)C4-C5	12.78	0.22	0.047

47.BD(2)C7-C8	96.BD*(2)C9-C10	17.19	0.21	0.053
47.BD(2)C7-C8	102.BD*(1)B15-C19	2.18	0.54	0.031
47.BD(2)C7-C8	103.BD*(1)B15-C20	2.20	0.54	0.031
47.BD(2)C7-C8	225.RY(3)C5	0.69	0.84	0.021
47.BD(2)C7-C8	328.RY(2)C9	1.63	0.72	0.031
48.BD(1)C7-B15	84.BD*(1)C4-C5	3.64	0.77	0.047
48.BD(1)C7-B15	93.BD*(1)C8-C9	5.34	0.82	0.059
48.BD(1)C7-B15	94.BD*(1)C8-H16	0.78	0.70	0.021
48.BD(1)C7-B15	106.BD*(1)C19-H24	1.55	0.69	0.029
48.BD(1)C7-B15	110.BD*(1)C20-H34	1.47	0.69	0.028
48.BD(1)C7-B15	118.BD*(1)As35-H37	1.44	0.47	0.023
48.BD(1)C7-B15	223.RY(1)C5	1.17	1.68	0.040
48.BD(1)C7-B15	224.RY(2)C5	1.58	1.67	0.046
48.BD(1)C7-B15	301.RY(1)C8	1.51	1.64	0.044
49.BD(1)C8-C9	90.BD*(1)C7-C8	1.03	1.02	0.029
49.BD(1)C8-C9	92.BD*(1)C7-B15	2.16	0.86	0.039
49.BD(1)C8-C9	95.BD*(1)C9-C10	0.95	1.03	0.028
49.BD(1)C8-C9	98.BD*(1)C10-H18	2.88	0.85	0.044
49.BD(1)C8-C9	275.RY(1)C7	1.44	1.87	0.046
49.BD(1)C8-C9	280.RY(6)C7	0.57	3.29	0.039
49.BD(1)C8-C9	353.RY(1)C10	0.70	2.00	0.033
50.BD(1)C8-H16	88.BD*(1)C5-C7	5.28	0.86	0.060
50.BD(1)C8-H16	95.BD*(1)C9-C10	3.68	0.92	0.052
50.BD(1)C8-H16	97.BD*(1)C9-H17	0.64	0.75	0.019
50.BD(1)C8-H16	104.BD*(1)B15-As35	0.87	0.56	0.020
50.BD(1)C8-H16	275.RY(1)C7	1.87	1.76	0.051
50.BD(1)C8-H16	327.RY(1)C9	1.08	1.83	0.040
51.BD(1)C9-C10	82.BD*(1)C3-C4	2.51	0.99	0.044
51.BD(1)C9-C10	86.BD*(1)C4-C10	0.90	0.99	0.027
51.BD(1)C9-C10	93.BD*(1)C8-C9	1.02	1.01	0.029
51.BD(1)C9-C10	94.BD*(1)C8-H16	2.10	0.89	0.039
51.BD(1)C9-C10	197.RY(1)C4	0.69	1.83	0.032
51.BD(1)C9-C10	198.RY(2)C4	0.85	2.08	0.038
51.BD(1)C9-C10	301.RY(1)C8	1.07	1.83	0.039
52.BD(2)C9-C10	85.BD*(2)C4-C5	14.06	0.24	0.052
52.BD(2)C9-C10	91.BD*(2)C7-C8	11.74	0.26	0.049
52.BD(2)C9-C10	199.RY(3)C4	0.50	0.79	0.018
52.BD(2)C9-C10	302.RY(2)C8	1.01	0.75	0.025
53.BD(1)C9-H17	86.BD*(1)C4-C10	3.98	0.89	0.053
53.BD(1)C9-H17	90.BD*(1)C7-C8	4.19	0.94	0.056
53.BD(1)C9-H17	94.BD*(1)C8-H16	0.55	0.79	0.019
53.BD(1)C9-H17	98.BD*(1)C10-H18	0.55	0.77	0.018
53.BD(1)C9-H17	301.RY(1)C8	1.08	1.73	0.039
53.BD(1)C9-H17	305.RY(5)C8	0.52	3.51	0.038
53.BD(1)C9-H17	353.RY(1)C10	1.24	1.91	0.044
54.BD(1)C10-H18	84.BD*(1)C4-C5	4.77	0.86	0.057
54.BD(1)C10-H18	93.BD*(1)C8-C9	3.76	0.91	0.052
54.BD(1)C10-H18	97.BD*(1)C9-H17	0.57	0.77	0.019
54.BD(1)C10-H18	197.RY(1)C4	0.52	1.73	0.027
54.BD(1)C10-H18	198.RY(2)C4	1.09	1.98	0.041
54.BD(1)C10-H18	327.RY(1)C9	1.20	1.85	0.042
55.BD(1)B14-C21	87.BD*(1)C5-C6	2.88	0.80	0.043
55.BD(1)B14-C21	89.BD*(1)C6-B14	0.51	0.71	0.017
55.BD(1)B14-C21	111.BD*(1)C21-H26	0.51	0.71	0.017
55.BD(1)B14-C21	112.BD*(1)C21-H27	0.63	0.71	0.019
55.BD(1)B14-C21	114.BD*(1)C22-H29	1.59	0.73	0.030
56.BD(1)B14-C22	76.BD*(1)C1-C6	0.70	0.86	0.022
56.BD(1)B14-C22	77.BD*(2)C1-C6	3.61	0.37	0.033
56.BD(1)B14-C22	111.BD*(1)C21-H26	1.88	0.70	0.032
56.BD(1)B14-C22	114.BD*(1)C22-H29	0.52	0.72	0.017
56.BD(1)B14-C22	117.BD*(1)As35-H36	1.75	0.47	0.026
57.BD(1)B14-As35	76.BD*(1)C1-C6	2.42	0.84	0.040
57.BD(1)B14-As35	77.BD*(2)C1-C6	1.94	0.35	0.023
57.BD(1)B14-As35	103.BD*(1)B15-C20	1.00	0.66	0.023
57.BD(1)B14-As35	104.BD*(1)B15-As35	1.03	0.48	0.020
57.BD(1)B14-As35	113.BD*(1)C21-H28	2.84	0.67	0.039
57.BD(1)B14-As35	115.BD*(1)C22-H30	2.56	0.68	0.037
57.BD(1)B14-As35	117.BD*(1)As35-H36	1.47	0.46	0.023
57.BD(1)B14-As35	118.BD*(1)As35-H37	1.71	0.46	0.025
57.BD(1)B14-As35	250.RY(2)C6	0.63	1.52	0.028
57.BD(1)B14-As35	587.RY(1)C22	0.80	1.24	0.028
58.BD(1)B15-C19	88.BD*(1)C5-C7	1.87	0.80	0.035
58.BD(1)B15-C19	91.BD*(2)C7-C8	1.59	0.38	0.022

58.BD(1)B15-C19	105.BD*(1)C19-H23	0.51	0.72	0.017
58.BD(1)B15-C19	106.BD*(1)C19-H24	0.54	0.70	0.017
58.BD(1)B15-C19	108.BD*(1)C20-H32	1.76	0.71	0.032
58.BD(1)B15-C19	117.BD*(1)As35-H36	1.36	0.48	0.023
59.BD(1)B15-C20	88.BD*(1)C5-C7	1.91	0.80	0.035
59.BD(1)B15-C20	91.BD*(2)C7-C8	1.93	0.37	0.024
59.BD(1)B15-C20	105.BD*(1)C19-H23	1.81	0.71	0.032
59.BD(1)B15-C20	110.BD*(1)C20-H34	0.55	0.70	0.017
60.BD(1)B15-As35	90.BD*(1)C7-C8	2.86	0.83	0.044
60.BD(1)B15-As35	99.BD*(1)B14-C21	1.40	0.67	0.027
60.BD(1)B15-As35	101.BD*(1)B14-As35	1.01	0.47	0.020
60.BD(1)B15-As35	107.BD*(1)C19-H25	2.73	0.68	0.038
60.BD(1)B15-As35	109.BD*(1)C20-H33	2.78	0.68	0.039
60.BD(1)B15-As35	117.BD*(1)As35-H36	1.52	0.46	0.024
60.BD(1)B15-As35	118.BD*(1)As35-H37	1.61	0.46	0.024
60.BD(1)B15-As35	276.RY(2)C7	0.72	1.41	0.028
60.BD(1)B15-As35	509.RY(1)C19	0.79	1.31	0.029
60.BD(1)B15-As35	535.RY(1)C20	0.69	1.25	0.026
61.BD(1)C19-H23	103.BD*(1)B15-C20	1.97	0.72	0.034
61.BD(1)C19-H23	444.RY(1)B15	1.05	1.48	0.035
62.BD(1)C19-H24	92.BD*(1)C7-B15	2.46	0.73	0.038
62.BD(1)C19-H24	445.RY(2)B15	0.93	1.43	0.033
63.BD(1)C19-H25	102.BD*(1)B15-C19	0.82	0.71	0.022
63.BD(1)C19-H25	104.BD*(1)B15-As35	2.94	0.53	0.035
63.BD(1)C19-H25	448.RY(5)B15	0.53	2.07	0.029
64.BD(1)C20-H32	102.BD*(1)B15-C19	2.12	0.71	0.035
64.BD(1)C20-H32	444.RY(1)B15	1.08	1.48	0.036
65.BD(1)C20-H33	103.BD*(1)B15-C20	0.70	0.72	0.020
65.BD(1)C20-H33	104.BD*(1)B15-As35	2.76	0.53	0.034
65.BD(1)C20-H33	447.RY(4)B15	0.56	1.80	0.028
66.BD(1)C20-H34	92.BD*(1)C7-B15	2.43	0.73	0.038
66.BD(1)C20-H34	446.RY(3)B15	0.76	1.68	0.032
67.BD(1)C21-H26	100.BD*(1)B14-C22	2.19	0.72	0.035
67.BD(1)C21-H26	418.RY(1)B14	0.62	1.50	0.027
67.BD(1)C21-H26	419.RY(2)B14	0.62	1.59	0.028
68.BD(1)C21-H27	89.BD*(1)C6-B14	2.87	0.74	0.041
68.BD(1)C21-H27	99.BD*(1)B14-C21	0.63	0.73	0.019
69.BD(1)C21-H28	99.BD*(1)B14-C21	0.66	0.73	0.020
69.BD(1)C21-H28	101.BD*(1)B14-As35	2.96	0.53	0.035
69.BD(1)C21-H28	420.RY(3)B14	0.56	1.75	0.028
70.BD(1)C22-H29	99.BD*(1)B14-C21	1.95	0.72	0.034
70.BD(1)C22-H29	419.RY(2)B14	0.92	1.58	0.034
71.BD(1)C22-H30	100.BD*(1)B14-C22	0.88	0.71	0.022
71.BD(1)C22-H30	101.BD*(1)B14-As35	3.19	0.53	0.037
72.BD(1)C22-H31	89.BD*(1)C6-B14	2.13	0.74	0.035
72.BD(1)C22-H31	421.RY(4)B14	0.88	1.98	0.037
73.BD(1)As35-H36	100.BD*(1)B14-C22	0.99	0.71	0.024
73.BD(1)As35-H36	101.BD*(1)B14-As35	1.69	0.53	0.027
73.BD(1)As35-H36	102.BD*(1)B15-C19	0.72	0.71	0.020
73.BD(1)As35-H36	104.BD*(1)B15-As35	1.82	0.53	0.028
73.BD(1)As35-H36	118.BD*(1)As35-H37	1.45	0.51	0.024
74.BD(1)As35-H37	89.BD*(1)C6-B14	0.71	0.73	0.020
74.BD(1)As35-H37	92.BD*(1)C7-B15	0.75	0.73	0.021
74.BD(1)As35-H37	101.BD*(1)B14-As35	2.08	0.53	0.030
74.BD(1)As35-H37	104.BD*(1)B15-As35	1.74	0.53	0.027
74.BD(1)As35-H37	117.BD*(1)As35-H36	1.41	0.51	0.024

Table S32. Natural Bond Orbitals Summary for [**1**-AsH]$^{-}$.Without Rydberg orbitals

NBO	Occupancy	Energy / a.u.	Principal delocalizations (geminal,vicinal,remote)
1.CR(1)C1	1.99998	-9.74713	
2.CR(1)C2	1.99998	-9.75989	
3.CR(1)C3	1.99998	-9.75903	
4.CR(1)C4	1.99998	-9.76589	
5.CR(1)C5	1.99998	-9.76435	
6.CR(1)C6	1.99998	-9.74062	
7.CR(1)C7	1.99998	-9.74096	
8.CR(1)C8	1.99998	-9.74772	
9.CR(1)C9	1.99998	-9.75983	
10.CR(1)C10	1.99998	-9.75834	
11.CR(1)B14	1.99996	-6.31932	
12.CR(1)B15	1.99996	-6.32113	
13.CR(1)C19	1.99998	-9.71486	
14.CR(1)C20	1.99998	-9.71418	
15.CR(1)C21	1.99998	-9.71524	
16.CR(1)C22	1.99998	-9.71259	
17.CR(1)As35	2.00000	-411.07221	
18.CR(2)As35	2.00000	-58.34135	
19.CR(3)As35	1.99998	-14.21158	
20.CR(4)As35	2.00000	-26.83156	
21.CR(5)As35	1.99999	-25.29326	
22.CR(6)As35	2.00000	-26.83450	
23.CR(7)As35	1.99999	-25.29728	
24.CR(8)As35	2.00000	-26.83451	
25.CR(9)As35	2.00000	-25.29730	
26.CR(10)As35	1.99996	-1.36312	
27.CR(11)As35	1.99996	-1.36303	
28.CR(12)As35	1.99997	-1.36692	
29.CR(13)As35	1.99994	-1.36326	
30.CR(14)As35	1.99992	-1.36618	
31.BD(1)C1-C2	1.98142	-0.38784	83(v),89(v),249(v),76(g)
			79(g),171(v),254(v)
32.BD(1)C1-C6	1.97384	-0.37857	88(v),81(v),89(g),223(v)
			75(g),101(v),87(g),145(v)
			418(v),147(v),78(g),224(v)
33.BD(2)C1-C6	1.69377	-0.08426	80(v),85(v),100(v),101(v)
			146(v),225(v)
34.BD(1)C1-H11	1.97231	-0.28174	87(v),79(v),249(v),145(v)
			250(v),112(r),81(v)
35.BD(1)C2-C3	1.98369	-0.40845	86(v),78(v),119(v),75(g)
			82(g),198(v),197(v)
36.BD(2)C2-C3	1.76431	-0.10699	85(v),77(v),120(v),199(v)
37.BD(1)C2-H12	1.97842	-0.30448	76(v),82(v),171(v),119(v)
			83(v),78(v)
38.BD(1)C3-C4	1.97587	-0.38496	81(v),88(v),95(v),223(v)
			353(v),79(g),84(g),86(g)
			145(v),147(v)
39.BD(1)C3-H13	1.97686	-0.30400	84(v),75(v),145(v),198(v)
			81(v),197(v)
40.BD(1)C4-C5	1.96709	-0.36342	92(v),89(v),98(v),83(v)
			249(v),275(v),86(g),82(g)
			88(g),87(g),355(v),173(v)
41.BD(2)C4-C5	1.52255	-0.07966	96(v),80(v),91(v),77(v)
			354(v),172(v),277(v),225(g)
42.BD(1)C4-C10	1.97595	-0.38561	97(v),87(v),79(v),223(v)
			171(v),95(g),84(g),82(g)
			327(v),329(v)
43.BD(1)C5-C6	1.97245	-0.35733	78(v),86(v),90(v),197(v)
			88(g),89(g),119(v),275(v)
			84(g)
44.BD(1)C5-C7	1.97300	-0.36078	94(v),82(v),76(v),197(v)
			87(g),301(v),249(v),92(g)
			84(g),90(g)
45.BD(1)C6-B14	1.93602	-0.22009	75(v),84(v),118(v),116(v)
			119(v),223(v),224(v),112(v)
			78(v)
46.BD(1)C7-C8	1.97182	-0.37600	87(v),97(v),92(g),104(v)
			93(g),223(v),224(v),88(g)
			327(v),329(v)

47.BD(2)C7-C8	1.67955	-0.08248	96(v),85(v),103(v),102(v)
			328(v),225(v)
48.BD(1)C7-B15	1.93999	-0.21744	93(v),84(v),224(v),106(v)
			301(v),110(v),118(v),223(v)
			94(v)
49.BD(1)C8-C9	1.98144	-0.38991	98(v),92(v),275(v),90(g)
			95(g),353(v),280(v)
50.BD(1)C8-H16	1.97206	-0.28272	88(v),95(v),275(v),327(v)
			104(r),97(v)
51.BD(1)C9-C10	1.98328	-0.40702	82(v),94(v),301(v),93(g)
			86(g),198(v),197(v)
52.BD(2)C9-C10	1.75528	-0.10607	85(v),91(v),302(v),199(v)
53.BD(1)C9-H17	1.97831	-0.30432	90(v),86(v),353(v),301(v)
			94(v),98(v),305(v)
54.BD(1)C10-H18	1.97687	-0.30374	84(v),93(v),327(v),198(v)
			97(v),197(v)
55.BD(1)B14-C21	1.97736	-0.22802	87(v),114(v),112(g),111(g)
			89(g)
56.BD(1)B14-C22	1.95073	-0.22011	77(v),111(v),117(v),76(v)
			114(g)
57.BD(1)B14-As35	1.94138	-0.20178	113(v),115(v),76(v),77(v)
			118(g),117(g),104(g),103(v)
			587(v),250(v)
58.BD(1)B15-C19	1.96224	-0.22422	88(v),108(v),91(v),117(v)
			106(g),105(g)
59.BD(1)B15-C20	1.96418	-0.22305	91(v),88(v),105(v),110(g)
60.BD(1)B15-As35	1.95186	-0.20240	90(v),109(v),107(v),118(g)
			117(g),99(v),101(g),509(v)
			276(v),535(v)
61.BD(1)C19-H23	1.98753	-0.25943	103(v),444(v)
62.BD(1)C19-H24	1.98629	-0.25897	92(v),445(v)
63.BD(1)C19-H25	1.97968	-0.25844	104(v),102(g),448(v)
64.BD(1)C20-H32	1.98835	-0.25801	102(v),444(v)
65.BD(1)C20-H33	1.98196	-0.25859	104(v),103(g),447(v)
66.BD(1)C20-H34	1.98495	-0.25875	92(v),446(v)
67.BD(1)C21-H26	1.98811	-0.26136	100(v),419(v),418(v)
68.BD(1)C21-H27	1.98575	-0.26009	89(v),99(g)
69.BD(1)C21-H28	1.98273	-0.26074	101(v),99(g),420(v)
70.BD(1)C22-H29	1.98670	-0.25634	99(v),419(v)
71.BD(1)C22-H30	1.97953	-0.25442	101(v),100(g)
72.BD(1)C22-H31	1.98572	-0.25784	89(v),421(v)
73.BD(1)As35-H36	1.98110	-0.25335	104(g),101(g),118(g),100(v)
			102(v)
74.BD(1)As35-H37	1.98002	-0.25533	101(g),104(g),117(g),92(v)
			89(v)
------non-Lewis----------			
75.BD*(1)C1-C2	0.02042	0.60149	
76.BD*(1)C1-C6	0.02055	0.63982	
77.BD*(2)C1-C6	0.25983	0.15014	
78.BD*(1)C1-H11	0.02070	0.49167	
79.BD*(1)C2-C3	0.01348	0.63988	
80.BD*(2)C2-C3	0.30023	0.12538	
81.BD*(1)C2-H12	0.01785	0.46398	
82.BD*(1)C3-C4	0.02057	0.57989	
83.BD*(1)C3-H13	0.01864	0.46250	
84.BD*(1)C4-C5	0.03909	0.55405	
85.BD*(2)C4-C5	0.47029	0.13548	
86.BD*(1)C4-C10	0.02039	0.58312	
87.BD*(1)C5-C6	0.03030	0.57011	
88.BD*(1)C5-C7	0.03094	0.57699	
89.BD*(1)C6-B14	0.03039	0.47783	
90.BD*(1)C7-C8	0.02023	0.63070	
91.BD*(2)C7-C8	0.25842	0.15084	
92.BD*(1)C7-B15	0.03102	0.47197	
93.BD*(1)C8-C9	0.02056	0.60741	
94.BD*(1)C8-H16	0.02136	0.48467	
95.BD*(1)C9-C10	0.01357	0.63751	
96.BD*(2)C9-C10	0.31167	0.12556	
97.BD*(1)C9-H17	0.01796	0.46387	
98.BD*(1)C10-H18	0.01859	0.46271	
99.BD*(1)B14-C21	0.01740	0.46815	
100.BD*(1)B14-C22	0.02178	0.45541	
101.BD*(1)B14-As35	0.05243	0.27198	

102.BD*(1)B15-C19	0.01959	0.45554	
103.BD*(1)B15-C20	0.02068	0.45828	
104.BD*(1)B15-As35	0.04535	0.27375	
105.BD*(1)C19-H23	0.00788	0.49103	
106.BD*(1)C19-H24	0.00833	0.47558	
107.BD*(1)C19-H25	0.01119	0.47558	
108.BD*(1)C20-H32	0.00717	0.48261	
109.BD*(1)C20-H33	0.01241	0.47600	
110.BD*(1)C20-H34	0.00774	0.47604	
111.BD*(1)C21-H26	0.00762	0.47806	
112.BD*(1)C21-H27	0.00737	0.48023	
113.BD*(1)C21-H28	0.01298	0.47043	
114.BD*(1)C22-H29	0.00714	0.49958	
115.BD*(1)C22-H30	0.01036	0.47783	
116.BD*(1)C22-H31	0.00810	0.47805	
117.BD*(1)As35-H36	0.03829	0.25475	
118.BD*(1)As35-H37	0.04568	0.25405	

QTAIM analyses were performed on the PBE0(D3BJ)/def2-TZVPP electron densities, using the AIMAll software with default integration.[7] To describe and compare the nature of chemical bonds, a variety of descriptors have been developed in the context of Bader's theory of AIM, specifically at the so-called bond critical points (BCP).[8] The components considered in the QTAIM analysis are the electron density, ρ(bcp) and the Laplacian of the density, $-\nabla^2 \rho$(bcp) Low electron densities and positive Laplacians are an indication for closed shell (ionic) interactions whereas the opposite is found for shared (covalent) bonds. Selected values are listed below. The electron density at the bondcritical point, ρ(bcp), as well as the Laplacian function, $-\nabla^2 \rho$(bcp), are given in atomic units and the ellipticity ε is dimensionless.

Table S33. Calculated atomic charges of **1** according to QTAIM.

1	
Atom	Charge, q
C1	-9.6359955000E-03
C2	-7.7762443000E-03
C3	-6.1802935470E-01
C4	-6.1813934480E-01
C5	-3.6468062000E-02
C6	-3.6477639600E-02
C7	-2.4049396000E-02
C8	-2.3941134700E-02
C9	-2.2241125500E-02
C10	-2.2248809800E-02
B11	1.8879004749E+00
B12	1.8878386417E+00
C13	-6.4890208920E-01
H14	1.9160757860E-02
H15	8.5048523500E-03
H16	2.7081596100E-03
C17	-6.4291326460E-01
H18	1.8011145430E-02
H19	4.1682706200E-03
H20	-5.0299061000E-03
C21	-6.4881092470E-01
H22	1.9156399850E-02
H23	8.5352938700E-03
H24	2.7061912300E-03
C25	-6.4247974670E-01
H26	1.7978790500E-02
H27	4.1782196200E-03
H28	-5.0903841000E-03
H29	1.9154345750E-02
H30	1.9215191630E-02
H31	2.4033576650E-02
H32	2.4032307020E-02
H33	2.2600393910E-02
H34	2.2599861940E-02
Total	2.4945214000E-04

Table S34. Calculated atomic charges of [**1**-OH]$^-$, [**1**-SH]$^-$. [**1**-SeH]$^-$ according to QTAIM.

[**1**-OH]$^-$		[**1**-SH]$^-$		[**1**-SeH]$^-$	
Atom	Charge, q	Atom	Atom	Charge, q	Atom
C1	-5.5223655800E-02	C1	-5.0131111100E-02	C1	-4.9796247800E-02
C2	-5.0351511200E-02	C2	-4.8898198300E-02	C2	-4.8303617500E-02
C3	-5.2017869000E-02	C3	-4.9905003200E-02	C3	-4.8954061400E-02
C4	-1.8847701800E-02	C4	-1.8366132400E-02	C4	-1.8375350600E-02
C5	-3.5593955000E-02	C5	-2.9395445000E-02	C5	-2.6640191800E-02
C6	-4.8834360490E-01	C6	-4.8270882180E-01	C6	-4.8934891060E-01
C7	-4.8826640780E-01	C7	-4.9358139830E-01	C7	-5.0576799530E-01
C8	-5.5256674800E-02	C8	-5.6501631200E-02	C8	-5.6479405500E-02
C9	-5.0276409600E-02	C9	-5.1079139700E-02	C9	-5.0829034100E-02
C10	-5.1997941100E-02	C10	-4.9621928600E-02	C10	-4.9229733900E-02
H11	-1.6556563300E-02	H11	-1.2775012300E-02	H11	-1.2071368600E-02
H12	-2.0296700600E-02	H12	-1.8005971000E-02	H12	-1.7335823800E-02
H13	-1.9481233800E-02	H13	-1.7910277500E-02	H13	-1.7293965500E-02
B14	1.9026378602E+00	B14	1.7270987874E+00	B14	1.6552009791E+00
B15	1.9023457953E+00	B15	1.7365657309E+00	B15	1.6711074048E+00
H16	-1.6606329000E-02	H16	-5.6785866000E-03	H16	-3.5461467000E-03
H17	-2.0298310700E-02	H17	-1.8829379000E-02	H17	-1.8272693300E-02
H18	-1.9481291200E-02	H18	-1.7893257000E-02	H18	-1.7307289300E-02
C19	-5.0795650240E-01	C19	-5.0583222590E-01	C19	-5.1928487590E-01
C20	-5.1102272270E-01	C20	-5.1241161310E-01	C20	-5.2593270940E-01
C21	-5.1087601450E-01	C21	-4.9611311410E-01	C21	-5.0691049440E-01
C22	-5.0785169770E-01	C22	-5.0770468200E-01	C22	-5.2076148970E-01
H23	-5.8554718200E-02	H23	-2.2517869100E-02	H23	-1.8316087600E-02
H24	-4.8887683000E-02	H24	-4.5998787700E-02	H24	-4.7001965700E-02
H25	-3.9447826400E-02	H25	-3.9220671700E-02	H25	-3.7805806000E-02
H26	-3.2889869200E-02	H26	-4.5636713600E-02	H26	-4.1440211800E-02
H27	-4.8142760600E-02	H27	-4.6699314000E-02	H27	-4.6412614300E-02
H28	-4.7982975800E-02	H28	-4.3691874600E-02	H28	-4.4155442400E-02
H29	-5.8572331600E-02	H29	-2.9199079200E-02	H29	-2.8927863600E-02
H30	-3.9485916600E-02	H30	-4.3876098700E-02	H30	-4.2878454000E-02
H31	-4.8866062600E-02	H31	-4.6199175200E-02	H31	-4.5397320500E-02
H32	-3.2859852800E-02	H32	-4.8690439300E-02	H32	-4.6328494700E-02
H33	-4.7992685000E-02	H33	-4.8076157100E-02	H33	-4.7800976200E-02
H34	-4.8162977500E-02	H34	-4.1823087800E-02	H34	-4.1479609800E-02
O35	-1.3286007381E+00	S35	-4.6496415700E-01	Se35	-2.0632492300E-01
H36	5.7151009607E-01	H36	-5.3377984000E-02	H36	-1.2927158770E-01
Total	-1.0005557427E+00	Total	-9.9964981880E-01	Total	-9.9967437850E-01

Table S35. Calculated atomic charges of [**1**-NH_2]$^-$, [**1**- PH_2]$^-$. [**1**- AsH_2]$^-$ according to QTAIM.

[**1**-NH_2]$^-$		[**1**-PH_2]$^-$		[**1**-AsH_2]$^-$	
Atom	Charge, q	Atom	Charge, q	Atom	Charge, q
C1	-5.5139096600E-02	C1	-5.3522405100E-02	C1	-5.3620145200E-02
C2	-5.1419990300E-02	C2	-5.0660858600E-02	C2	-5.0313768400E-02
C3	-5.2686702600E-02	C3	-4.9051423600E-02	C3	-4.8252137600E-02
C4	-1.9462781900E-02	C4	-1.8463673500E-02	C4	-1.7734708900E-02
C5	-3.7932946800E-02	C5	-3.1408033200E-02	C5	-3.0671299300E-02
C6	-4.7664365390E-01	C6	-4.7420297670E-01	C6	-4.9192742670E-01
C7	-4.7686160180E-01	C7	-4.6252861120E-01	C7	-4.7385613600E-01
C8	-5.5242725500E-02	C8	-4.7871703300E-02	C8	-4.7505557800E-02
C9	-5.1483639700E-02	C9	-4.9310977100E-02	C9	-4.8535665600E-02
C10	-5.2806607100E-02	C10	-4.9553514600E-02	C10	-4.8726754600E-02
H11	-1.4943519400E-02	H11	-3.0791421000E-03	H11	-1.3559726000E-03
H12	-2.1376074400E-02	H12	-1.8678655800E-02	H12	-1.7940434300E-02
H13	-2.0449252900E-02	H13	-1.7895506700E-02	H13	-1.7178783700E-02
B14	1.8620597482E+00	B14	1.6295419590E+00	B14	1.5850857718E+00
B15	1.8626629207E+00	B15	1.6218082999E+00	B15	1.5700691163E+00
H16	-1.4989045000E-02	H16	-1.1018511500E-02	H16	-1.0506043100E-02
H17	-2.1379039600E-02	H17	-1.8086680000E-02	H17	-1.7293192000E-02
H18	-2.0450157400E-02	H18	-1.8033855000E-02	H18	-1.7357134800E-02
C19	-4.9081624540E-01	C19	-4.8985368860E-01	C19	-5.0599941720E-01
C20	-4.9390992500E-01	C20	-4.8515709600E-01	C20	-4.9927149950E-01
C21	-4.9370146660E-01	C21	-5.0375183010E-01	C21	-5.1964251330E-01
C22	-4.9118879030E-01	C22	-4.8482918670E-01	C22	-5.0261944800E-01
H23	-5.9054220900E-02	H23	-3.1083972600E-02	H23	-3.2240475700E-02
H24	-6.4341750700E-02	H24	-5.2023322000E-02	H24	-4.9613728900E-02
H25	-4.7744660300E-02	H25	-4.3862883800E-02	H25	-4.4085052200E-02
H26	-3.2493072600E-02	H26	-4.6883620300E-02	H26	-4.6089798200E-02
H27	-6.5925160200E-02	H27	-4.9300464500E-02	H27	-4.6781867600E-02
H28	-4.6214922000E-02	H28	-5.0238906200E-02	H28	-4.9659478200E-02
H29	-5.9052714200E-02	H29	-2.2093140800E-02	H29	-1.9937501300E-02
H30	-4.7692868200E-02	H30	-3.9480266600E-02	H30	-3.8302363300E-02
H31	-6.4344574100E-02	H31	-5.1198089200E-02	H31	-5.0059242400E-02
H32	-3.2531852300E-02	H32	-4.3365729800E-02	H32	-4.1457677000E-02
H33	-4.6220017700E-02	H33	-4.8462600800E-02	H33	-4.7863507200E-02
H34	-6.5926627200E-02	H34	-5.3743373600E-02	H34	-5.1781798800E-02
N35	-1.3438367347E+00	P35	6.3187775800E-01	As35	3.7975372500E-01
H36	3.3446560988E-01	H36	-5.0618736410E-01	H36	-2.9626184160E-01
H37	3.2957879338E-01	H37	-5.0948403710E-01	H37	-3.0053550060E-01
Total	-9.9949536514E-01	Total	-1.0011380839E+00	Total	-1.0000692585E+00

Table S36. Characteristic parameters from the electron density topology of **1**.

BCP Number	Atom pair	ρ(bcp)	$-\nabla^2 \rho$(bcp)	ε
BCP1	C1-C2	0.290294	+0.779322	0.144531
BCP2	C1-C3	0.287819	+0.767200	0.123023
BCP3	C1-C4	0.287820	+0.767206	0.123024
BCP4	C7-C9	0.322982	+0.928092	0.214377
BCP5	C3-C5	0.309387	+0.853423	0.169795
BCP6	C5-H29	0.282777	+1.015859	0.015800
BCP7	C8-C10	0.322982	+0.928092	0.214378
BCP8	C4-C6	0.309387	+0.853418	0.169796
BCP9	C6-H30	0.282776	+1.015853	0.015800
BCP10	C5-C7	0.303191	+0.844560	0.152664
BCP11	C6-C8	0.303191	+0.844560	0.152665
BCP12	C2-C9	0.299304	+0.828753	0.145320
BCP13	C2-C10	0.299304	+0.828752	0.145321
BCP14	C3-B11	0.185006	+0.238177	0.227833
BCP15	C4-B12	0.185007	+0.238178	0.227836
BCP16	C4-H15	0.010101	–0.030850	0.771127
BCP17	B11-C13	0.181307	+0.301622	0.212952
BCP18	C13-H15	0.272988	+0.932096	0.014905
BCP19	C13-H14	0.259871	+0.844999	0.032481
BCP20	C13-H16	0.268254	+0.900559	0.018287
BCP21	B11-C17	0.183286	+0.310772	0.209036
BCP22	C17-H18	0.263132	+0.866262	0.026767
BCP23	C17-H19	0.266570	+0.889003	0.021733
BCP24	C17-H20	0.271264	+0.919945	0.014467
BCP25	C3-H23	0.010099	–0.030847	0.772181
BCP26	B12-C21	0.181306	+0.301627	0.212959
BCP27	C21-H23	0.272989	+0.932096	0.014906
BCP28	C21-H22	0.259872	+0.845003	0.032480
BCP29	C21-H24	0.268254	+0.900560	0.018284
BCP30	B12-C25	0.183286	+0.310781	0.209044
BCP31	C25-H26	0.263138	+0.866298	0.026759
BCP32	C25-H27	0.266564	+0.888962	0.021740
BCP33	C25-H28	0.271266	+0.919956	0.014458
BCP34	C7-H31	0.282086	+1.012150	0.015404
BCP35	C8-H32	0.282086	+1.012150	0.015404
BCP36	C9-H33	0.281419	+1.007664	0.014195
BCP37	C10-H34	0.281419	+1.007663	0.014196

Table S37. Characteristic parameters from the electron density topology of [**1**-OH]$^{-}$.

BCP Number	Atom pair	ρ(bcp)	$-\nabla^2 \rho$(bcp)	ε
BCP1	C5-C6	0.286092	+0.755856	0.114087
BCP2	C1-C2	0.301875	+0.834537	0.166625
BCP3	C2-C3	0.321143	+0.915668	0.227280
BCP4	C4-C5	0.283603	+0.746082	0.139826
BCP5	C3-C4	0.298733	+0.821827	0.158145
BCP6	C1-C6	0.312068	+0.865719	0.168957
BCP7	C1-H11	0.278871	+0.983317	0.022855
BCP8	C4-C10	0.298731	+0.821818	0.158135
BCP9	C5-C7	0.286087	+0.755834	0.114068
BCP10	C9-C10	0.321147	+0.915684	0.227289
BCP11	C7-C8	0.312071	+0.865736	0.168972
BCP12	C8-H16	0.278874	+0.983336	0.022860
BCP13	C8-C9	0.301871	+0.834520	0.166609
BCP14	C2-H12	0.277705	+0.977675	0.017287
BCP15	C3-H13	0.276921	+0.969804	0.024031
BCP16	C6-B14	0.163773	+0.162791	0.199605
BCP17	C7-B15	0.163773	+0.162786	0.199574
BCP18	C9-H17	0.277705	+0.977674	0.017287
BCP19	C10-H18	0.276921	+0.969806	0.024029
BCP20	B15-C19	0.162835	+0.245150	0.153126
BCP21	B15-O35	0.114417	–0.405476	0.007751
BCP22	B15-C20	0.159556	+0.213544	0.147944
BCP23	B14-C21	0.159549	+0.213538	0.147966
BCP24	B14-O35	0.114421	–0.405488	0.007790
BCP25	B14-C22	0.162836	+0.245152	0.153112
BCP26	C21-H23	0.262849	+0.860382	0.023072
BCP27	C21-H24	0.264743	+0.872576	0.022208
BCP28	C21-H25	0.266387	+0.885183	0.022381
BCP29	C19-H26	0.268279	+0.897163	0.020582
BCP30	H26-H32	0.007573	–0.022698	0.275306
BCP31	C19-H27	0.265047	+0.876015	0.021189
BCP32	C19-H28	0.265170	+0.876128	0.023036
BCP33	C20-H29	0.262848	+0.860372	0.023073
BCP34	C20-H30	0.266384	+0.885162	0.022382
BCP35	C20-H31	0.264746	+0.872598	0.022210
BCP36	C22-H32	0.268280	+0.897172	0.020584
BCP37	C22-H33	0.265168	+0.876115	0.023037
BCP38	C22-H34	0.265046	+0.876008	0.021189
BCP39	O35-H36	0.367165	+2.676307	0.017610

Table S38. Characteristic parameters from the electron density topology of [**1**-SH]$^{-}$.

BCP Number	Atom pair	ρ(bcp)	$-\nabla^2 \rho$(bcp)	ε
BCP1	C5-C6	0.283630	+0.743046	0.123126
BCP2	C1-C2	0.303480	+0.842374	0.167090
BCP3	C2-C3	0.322265	+0.922806	0.224848
BCP4	C3-C4	0.299480	+0.825280	0.159027
BCP5	C4-C5	0.281994	+0.737002	0.142843
BCP6	C4-C10	0.298091	+0.819816	0.154701
BCP7	C1-C6	0.310132	+0.853892	0.169406
BCP8	C1-H11	0.279775	+0.989851	0.021622
BCP9	C5-C7	0.282109	+0.737549	0.115003
BCP10	C10-H18	0.277238	+0.972370	0.023059
BCP11	C9-C10	0.323526	+0.928030	0.228879
BCP12	C7-C8	0.311787	+0.862928	0.176613
BCP13	C8-H16	0.281097	+0.998145	0.024061
BCP14	C8-C9	0.301615	+0.834996	0.160100
BCP15	C3-H13	0.277230	+0.972136	0.023533
BCP16	C2-H12	0.277915	+0.979361	0.017286
BCP17	C6-B14	0.159748	+0.157607	0.142720
BCP18	C7-B15	0.162619	+0.151048	0.118783
BCP19	C9-H17	0.277806	+0.978446	0.017336
BCP20	B15-C19	0.159490	+0.226026	0.087155
BCP21	B15-C20	0.160491	+0.212515	0.087273
BCP22	B14-C21	0.158283	+0.215475	0.088899
BCP23	B14-C22	0.159959	+0.228131	0.081584
BCP24	H23-H29	0.008099	–0.024420	0.126736
BCP25	C19-H24	0.265496	+0.879117	0.016358
BCP26	C19-H23	0.269962	+0.908682	0.015683
BCP27	C19-H25	0.265210	+0.876600	0.020977
BCP28	C21-H26	0.266328	+0.885044	0.016670
BCP29	C21-H27	0.265883	+0.881801	0.017337
BCP30	C21-H28	0.265691	+0.880292	0.020452
BCP31	C22-H29	0.269124	+0.902906	0.015590
BCP32	C22-H30	0.265067	+0.875463	0.021038
BCP33	C22-H31	0.265921	+0.881602	0.016670
BCP34	C20-H32	0.265549	+0.879308	0.016908
BCP35	C20-H33	0.264677	+0.872318	0.020111
BCP36	C20-H34	0.266497	+0.885006	0.019036
BCP37	B14-S35	0.101121	+0.069878	0.063147
BCP38	B15-S35	0.099613	+0.065384	0.032558
BCP39	S35-H36	0.212638	+0.626508	0.030820

Table S39. Characteristic parameters from the electron density topology of [**1**-SeH]$^{-}$.

BCP Number	Atom pair	ρ(bcp)	$-\nabla^2 \rho$(bcp)	ε
BCP1	C5-C6	0.282914	+0.739448	0.124458
BCP2	C1-C2	0.303643	+0.843042	0.167187
BCP3	C2-C3	0.322528	+0.924320	0.224640
BCP4	C3-C4	0.299525	+0.825511	0.158978
BCP5	C3-H13	0.277317	+0.972821	0.023442
BCP6	C4-C5	0.281907	+0.736124	0.144137
BCP7	C1-C6	0.309372	+0.849034	0.169499
BCP8	C5-C7	0.281138	+0.733277	0.114751
BCP9	C4-C10	0.297856	+0.818868	0.153961
BCP10	C10-H18	0.277326	+0.973055	0.022938
BCP11	C9-C10	0.323909	+0.929985	0.229194
BCP12	C7-C8	0.311468	+0.861086	0.177813
BCP13	C8-C9	0.301597	+0.835108	0.159118
BCP14	C1-H11	0.279945	+0.990903	0.021475
BCP15	C2-H12	0.277977	+0.979835	0.017367
BCP16	C6-B14	0.159480	+0.164647	0.152834
BCP17	C7-B15	0.163685	+0.155333	0.117589
BCP18	C9-H17	0.277854	+0.978808	0.017397
BCP19	C8-H16	0.281485	+1.000829	0.024211
BCP20	B15-C19	0.160843	+0.229721	0.094066
BCP21	B15-C20	0.162265	+0.218879	0.096790
BCP22	B14-C21	0.159742	+0.224011	0.098234
BCP23	B14-C22	0.161017	+0.230849	0.086644
BCP24	H23-H29	0.008080	–0.024531	0.108692
BCP25	C19-H24	0.265471	+0.878937	0.015638
BCP26	C19-H23	0.270433	+0.912159	0.015208
BCP27	C19-H25	0.264543	+0.872349	0.021325
BCP28	C21-H26	0.267022	+0.890064	0.015943
BCP29	C21-H27	0.266134	+0.883782	0.016633
BCP30	C21-H28	0.265118	+0.876642	0.020541
BCP31	C22-H29	0.268983	+0.902146	0.014920
BCP32	C22-H30	0.264569	+0.872324	0.021210
BCP33	C22-H31	0.266078	+0.882654	0.016052
BCP34	C20-H32	0.265940	+0.882073	0.016411
BCP35	C20-H33	0.264003	+0.868074	0.020203
BCP36	C20-H34	0.266725	+0.886713	0.018986
BCP37	B14-Se35	0.088218	+0.104450	0.053607
BCP38	B15-Se35	0.086058	+0.093537	0.021663
BCP39	Se35-H36	0.171093	+0.287854	0.016730

Table S40. Characteristic parameters from the electron density topology of [**1**-NH_2]$^-$.

BCP Number	Atom pair	ρ(bcp)	$-\nabla^2\rho$(bcp)	ε
BCP1	C5-C6	0.285303	+0.751772	0.114221
BCP2	C1-C2	0.302011	+0.835468	0.166059
BCP3	C2-C3	0.321354	+0.916905	0.227226
BCP4	C4-C5	0.283163	+0.743793	0.139523
BCP5	C3-C4	0.298734	+0.821839	0.158153
BCP6	C1-C6	0.312253	+0.867570	0.169607
BCP7	C1-H11	0.279256	+0.985954	0.022948
BCP8	C4-C10	0.298734	+0.821839	0.158153
BCP9	C5-C7	0.285303	+0.751772	0.114221
BCP10	C9-C10	0.321354	+0.916905	0.227226
BCP11	C7-C8	0.312253	+0.867570	0.169607
BCP12	C8-H16	0.279256	+0.985954	0.022948
BCP13	C8-C9	0.302011	+0.835468	0.166059
BCP14	C2-H12	0.277584	+0.976777	0.017346
BCP15	C3-H13	0.276826	+0.969073	0.024068
BCP16	C6-B14	0.160961	+0.136791	0.134418
BCP17	C7-B15	0.160961	+0.136791	0.134418
BCP18	N35-H37	0.337550	+1.637920	0.012775
BCP19	C9-H17	0.277584	+0.976777	0.017346
BCP20	C10-H18	0.276826	+0.969073	0.024068
BCP21	B15-N35	0.132048	–0.227936	0.002102
BCP22	B15-C19	0.155249	+0.184861	0.096984
BCP23	B15-C20	0.157445	+0.206502	0.097573
BCP24	B14-C21	0.157445	+0.206502	0.097573
BCP25	B14-C22	0.155249	+0.184861	0.096984
BCP26	B14-N35	0.132048	–0.227936	0.002102
BCP27	C19-H23	0.263659	+0.866226	0.022015
BCP28	C19-H24	0.262614	+0.858427	0.023513
BCP29	C19-H25	0.266132	+0.883277	0.021800
BCP30	H26-H32	0.009127	–0.027105	0.258680
BCP31	C21-H26	0.269031	+0.902034	0.019128
BCP32	C21-H27	0.262060	+0.855519	0.021498
BCP33	C21-H28	0.265768	+0.880463	0.022027
BCP34	C22-H29	0.263659	+0.866226	0.022015
BCP35	C22-H30	0.266132	+0.883277	0.021800
BCP36	C22-H31	0.262614	+0.858427	0.023513
BCP37	C20-H32	0.269031	+0.902034	0.019128
BCP38	C20-H33	0.265768	+0.880463	0.022027
BCP39	C20-H34	0.262060	+0.855519	0.021498
BCP40	N35-H36	0.338483	+1.651192	0.009561

Table S41. Characteristic parameters from the electron density topology of [**1**-PH_2]$^-$.

BCP Number	Atom pair	ρ(bcp)	$-\nabla^2 \rho$(bcp)	ε
BCP1	C1-C2	0.301887	+0.836295	0.159961
BCP2	C2-C3	0.323831	+0.929980	0.228436
BCP3	C4-C5	0.281116	+0.732305	0.143207
BCP4	C3-C4	0.298156	+0.820031	0.154886
BCP5	C3-H13	0.277287	+0.972701	0.022989
BCP6	C1-C6	0.311983	+0.863949	0.177727
BCP7	C5-C6	0.279411	+0.723178	0.116170
BCP8	C6-B14	0.154318	+0.121987	0.063438
BCP9	C5-C7	0.281230	+0.730132	0.123922
BCP10	C7-B15	0.153021	+0.132926	0.063765
BCP11	C7-C8	0.310830	+0.857641	0.171457
BCP12	C4-C10	0.299357	+0.824732	0.158854
BCP13	C10-H18	0.277259	+0.972311	0.023499
BCP14	C9-C10	0.322682	+0.925151	0.224915
BCP15	C8-C9	0.303633	+0.843390	0.165979
BCP16	C8-H16	0.279956	+0.991525	0.021654
BCP17	C1-H11	0.281415	+1.000654	0.024259
BCP18	C2-H12	0.277792	+0.978416	0.017313
BCP19	B14-P35	0.118433	+0.188291	0.042361
BCP20	B14-C21	0.158206	+0.189519	0.024188
BCP21	B15-P35	0.117974	+0.193936	0.023546
BCP22	P35-H37	0.160750	+0.120273	0.082624
BCP23	C9-H17	0.277873	+0.979142	0.017194
BCP24	B15-C19	0.155368	+0.198770	0.022841
BCP25	B15-C20	0.155510	+0.194653	0.032260
BCP26	C21-H27	0.265544	+0.878669	0.018341
BCP27	B14-C22	0.154462	+0.199165	0.017434
BCP28	H23-H29	0.007763	–0.023298	0.127653
BCP29	C19-H23	0.269047	+0.902909	0.013951
BCP30	C19-H24	0.265397	+0.878149	0.015568
BCP31	C19-H25	0.264930	+0.875122	0.019950
BCP32	C21-H26	0.265959	+0.882356	0.016194
BCP33	C21-H28	0.264225	+0.869497	0.018884
BCP34	C22-H29	0.270222	+0.910938	0.014069
BCP35	C22-H30	0.265210	+0.877139	0.019548
BCP36	C22-H31	0.265365	+0.878361	0.014632
BCP37	C20-H34	0.265112	+0.876702	0.017001
BCP38	C20-H32	0.267046	+0.890131	0.015943
BCP39	C20-H33	0.265180	+0.876894	0.019553
BCP40	P35-H36	0.161846	+0.117968	0.084978

Table S42. Characteristic parameters from the electron density topology of [**1**-AsH_2]$^-$.

BCP Number	Atom pair	ρ(bcp)	$-\nabla^2\rho$(bcp)	ε
BCP1	C1-C2	0.302050	+0.837360	0.159063
BCP2	C2-C3	0.324265	+0.932338	0.228433
BCP3	C4-C5	0.280718	+0.729927	0.144306
BCP4	C3-C4	0.298030	+0.819585	0.154271
BCP5	C3-H13	0.277399	+0.973580	0.022788
BCP6	C1-C6	0.311546	+0.861508	0.177915
BCP7	C5-C6	0.277865	+0.715770	0.115617
BCP8	C6-B14	0.156131	+0.133128	0.071511
BCP9	C5-C7	0.280087	+0.724128	0.124554
BCP10	C7-B15	0.153485	+0.145837	0.093392
BCP11	C7-C8	0.310086	+0.852917	0.170885
BCP12	C4-C10	0.299413	+0.825010	0.158797
BCP13	C10-H18	0.277363	+0.973101	0.023400
BCP14	C9-C10	0.323050	+0.927285	0.224597
BCP15	C8-C9	0.303933	+0.844845	0.166000
BCP16	C8-H16	0.280139	+0.992601	0.021362
BCP17	C1-H11	0.281789	+1.003148	0.024183
BCP18	C2-H12	0.277866	+0.978968	0.017349
BCP19	B14-As35	0.100505	+0.143439	0.047413
BCP20	B14-C21	0.160864	+0.202834	0.047794
BCP21	B15-As35	0.100917	+0.149744	0.021100
BCP22	C9-H17	0.277952	+0.979753	0.017213
BCP23	B15-C19	0.157772	+0.209313	0.041831
BCP24	B15-C20	0.157835	+0.208309	0.055246
BCP25	C21-H27	0.266012	+0.881987	0.018601
BCP26	B14-C22	0.156913	+0.210264	0.040256
BCP27	H23-H29	0.007163	–0.021606	0.136518
BCP28	C19-H23	0.268597	+0.899982	0.014188
BCP29	C19-H24	0.265730	+0.880441	0.015622
BCP30	C19-H25	0.264458	+0.871982	0.020373
BCP31	C21-H26	0.266114	+0.883427	0.016053
BCP32	C21-H28	0.263777	+0.866624	0.019148
BCP33	C22-H29	0.270161	+0.910591	0.014282
BCP34	C22-H30	0.264659	+0.873546	0.020043
BCP35	C22-H31	0.265572	+0.879688	0.014418
BCP36	C20-H34	0.265529	+0.879677	0.016825
BCP37	C20-H32	0.267256	+0.891665	0.015730
BCP38	C20-H33	0.264874	+0.874980	0.019822
BCP39	As35-H36	0.146222	+0.100599	0.048568
BCP40	As35-H37	0.144908	+0.098778	0.051241

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