Supplementary Information

Synthesis of Digermylene-Stabilized Linear Tetraboronate and Boroxine

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General information

All manipulations were carried out on a Schlenk line or in an argon atomsphere glovebox. Solvents were dried by refluxing with sodium benzophenone under N_2, distilled, and stored over activated molecular sieves. Benzene-d6 were each dried over sodium and distilled prior to use. N-heterocyclic ylide-like germylene was prepared using literature methods.[1] Unless otherwise stated, commercial reagents were purchased from Sigma-Aldrich or Alfa and used without further purification. ^{1}H and ^{13}C NMR spectra were measured on Bruker 400MHz spectrometers. ^{1}H and ^{13}C NMR spectroscopic chemical shifts were given relative to residual solvent peaks. IR spectra were recorded on a Nicolet 330 spectrometer. Mass spectra were measured using Bruker Amazon SL ion trap mass spectrometer.

Experimental section:

*(L^1Ge[OB(Ph)]$_2$)$_2$O (**2**)* and *L^1GeOH (**5**)*:

At -78 °C, a solution of $PhB(OH)_2$ (0.122 g, 1 mmol) in toluene (15 mL) was added drop by drop to a solution of **1** (0.489 g, 1 mmol) in toluene/^{n}hexane (20 mL). The mixture was stirred and slowly warmed to 35 °C. After stirring for additional 24 h, the solvent was removed and the residue was extract with 10 mL ^{n}hexane. 3 mL toluene was added into the ^{n}hexane solution, and the mixture was then stored at -20 °C. Light yellow block crystals of **2** were isolate after 5 days (33 % yield according to **1**). Then the mother liquor was stored at -20 °C for another 2 weeks. A small amount of colorless crystals of **5** was obtained.

2: ^{1}H NMR (400 MHz, C_6D_6, ppm): δ 8.22-8.21 (m, 8 H, Ar*H*), 7.39-7.37 (m, 4 H, Ar*H*), 7.29-7.23 (m, 6 H, Ar*H*), 7.19-7.17 (m, 6 H, Ar*H*), 7.12-7.04 (m, 8 H, Ar*H*), 5.03 (s, 2 H, γ-*H*), 3.86 (sept, *J* = 6.8 Hz, 4 H, C*H*Me$_2$), 3.27 (sept, *J* = 6.7 Hz, 4 H, C*H*Me$_2$), 1.60 (s, 12 H, β-*Me*), 1.31 (d, *J* = 6.8 Hz, 12 H, CH*Me$_2$*), 1.26 (d, *J* = 6.8 Hz, 12 H, CH*Me$_2$*), 1.16 (d, *J* = 6.8 Hz, 12 H, CH*Me$_2$*), 1.11 (d, *J* = 6.2 Hz, 12 H, CH*Me$_2$*). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6, ppm): δ 163.60 (*C*N), 148.47, 147.94, 145.46, 143.29, 142.58, 141.46, 140.29, 127.16, 124.63, 123.69 (*Ar*), 95.90 (γ-*C*H), 29.46, 28.92 (*C*HMe$_2$), 27.49, 27.19, 26.65, 26.31 (CH*Me$_2$*), 24.38 (d, *J* = 1.5 Hz, β-*Me*). ^{11}B NMR (160 MHz, C_6D_6, ppm): δ 13.2 (br, $h_{1/2}$ = 810 Hz), Similar broad ^{11}B signals were reported, see references (N. F. McKinley, D. F. O'Shea, *J. Org. Chem.*, 2004, **69**, 5087-5092; C. Ma, J. Zhang, J. Li, C. Cui, *Chem. Comm.*, 2015, **51**, 5732-5734; and G. Vargas, I. Hernández, H. Höpfl, M.-E. Ochoa, D. Castillo, N. Farfán, R. Santillan, E. Gómez, *Inorg. Chem.*, 2004, **43**, 8490-8500). IR (Nujol mull, cm^{-1}): $\tilde{\nu}$ 1530.1, 1499.7, 1420.3, 1329.2, 1301.0, 1247.8, 1216.1, 1154.9, 1028.7, 971.5, 773.8, 720.7,

655.0, 639.1, 591.8, 547.6. ESI-MS: *m/z* = 1414 $[M + H]^+$. Elem. Anal. Calcd for $C_{82}H_{102}B_4Ge_2N_4O_5$: C, 69.74; H, 7.28; N, 3.97; Found: C, 70.02; H, 7.38; N, 3.91.

5: ^{1}H NMR (400 MHz, C_6D_6, ppm): δ 7.19-7.15 (m, 4 H, Ar*H*), 7.12-7.09 (m, 2 H, Ar*H*), 4.91 (s, 1 H, γ-*H*), 3.72 (sept, *J* = 6.8 Hz, 2 H, C*H*Me$_2$), 3.32 (sept, *J* = 6.9 Hz, 2 H, C*H*Me$_2$), 1.60 (s, 6 H, β-*Me*), 1.54 (s, 1 H, O*H*), 1.31 (d, *J* = 6.9 Hz, 6 H, CH*Me$_2$*, overlapped), 1.30 (d, *J* = 6.6 Hz, 6 H, CH*Me$_2$*, overlapped), 1.32 (d, *J* = 6.9 Hz, 6 H, CH*Me$_2$*), 1.12 (d, *J* = 6.9 Hz, 6 H, CH*Me$_2$*). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6, ppm): δ 163.33 (*C*N), 146.40, 143.65, 141.02, 127.47, 124.87, 124.06 (*Ar*), 96.98 (γ-*C*H), 29.16, 28.03 (*C*HMe$_2$), 26.67, 24.74, 24.56, 24.08 (CH*Me$_2$*), 23.25. IR (Nujol mull, cm^{-1}): $\tilde{\nu}$ 3566.9, 1556.4, 1527.8, 1458.3, 1380.7, 1315.3, 1258.1, 1176.4, 1098.8, 1017.0, 853.6, 792.3, 755.5, 588.0. ESI-MS: *m/z* = 508 $[M + H]^+$.

*L^{1}GeOB(2-Ph-C$_6$H$_4$)(OH) (**3**)*. At -20 °C, a solution of 2-Ph-$C_6H_4B(OH)_2$ (0.198 g, 1 mmol) in toluene (10 mL) was added dropwise into a solution of **1** (0.489 g, 1 mmol) in toluene (10 mL). The mixture was stirred and slowly warmed to room temperature for 12 h. Then the toluene was removed and the residue was wash with 10 mL ^{n}hexane for 2 times to get analytical pure **3** (78 % yield). Colorless block crystals of **3** suitable for X-ray single crystal test were obtained after 1 day from a toluene solution. ^{1}H NMR (400 MHz, C_6D_6, ppm): δ 8.35 (dd, *J* = 7.4, 1.3 Hz, 1 H, Ar*H*), 7.38-7.35 (m, 2 H, Ar*H*), 7.27 (td, *J* = 3.6, 1.6 Hz, 1 H, Ar*H*), 7.22 (td, *J* = 3.6, 1.6 Hz, 1 H, Ar*H*), 7.14-7.00 (m, 9 H, Ar*H*), 5.06 (s, 1 H, γ-*H*), 3.87 (s, 1 H, O*H*), 3.76 (sept, *J* = 6.8 Hz, 2 H, C*H*Me$_2$), 3.27 (sept, *J* = 6.7 Hz, 2 H, C*H*Me$_2$), 1.64 (s, 6 H, β-*Me*), 1.24 (d, *J* = 7.0 Hz, 6 H, CH*Me$_2$*, overlapped), 1.22 (d, *J* = 6.7 Hz, 6 H, CH*Me$_2$*, overlapped), 1.17 (d, *J* = 6.8 Hz, 6 H, CH*Me$_2$*), 1.10 (d, *J* = 6.8 Hz, 6 H, CH*Me$_2$*). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6, ppm): δ 162.98 (*C*N), 147.07, 145.44, 143.81,

142.77, 140.01, 136.09, 128.62, 128.33, 128.19, 127.51, 126.56, 126.30, 125.70, 123.94, 123.12 (*Ar*), 97.41 (γ-*C*H), 28.21, 26.95 (*C*HMe$_2$), 25.89 (β-*Me*), 23.84, 23.56, 23.26, 22.42 (CH*Me$_2$*). ^{11}B NMR (160 MHz, C_6D_6, ppm): δ 28.7 (br, $h_{1/2}$ = 690 Hz), Similar broad ^{11}B signals were reported, see references (N. F. McKinley, D. F. O'Shea, *J. Org. Chem.*, 2004, **69**, 5087-5092; C. Ma, J. Zhang, J. Li, C. Cui, *Chem. Comm.*, 2015, **51**, 5732-5734; and G. Vargas, I. Hernández, H. Höpfl, M.-E. Ochoa, D. Castillo, N. Farfán, R. Santillan, E. Gómez, *Inorg. Chem.*, 2004, **43**, 8490-8500). IR (Nujol mull, cm^{-1}): $\tilde{\nu}$ 3603.6, 1560.5, 1531.9, 1466.5, 1437.9, 1364.4, 1315.3, 1249.9, 1233.6, 1172.3, 1106.9, 1041.5, 857.7, 804.5, 767.8, 702.4, 649.3, 600.2, 534.9. ESI-MS: *m/z* = 688 [M + H]$^+$. Elem. Anal. Calcd for $C_{41}H_{51}BGeN_2O_2$: C, 71.65; H, 7.48; N, 4.08; Found: C, 71.75; H, 7.32; N, 4.13.

*MesB([OB(L^{1}Ge)]$_2$O) (**4**)* A solution of Mes$_2$B(OH) (0.198 g, 1 mmol) in toluene (10 mL) was added dropwise into a solution of **1** (0.489 g, 1 mmol) in toluene (10 mL) in room temperature. The mixture was stirred for 1 hour, then the solvent was removed and 20 mL ^{n}hexane was added in. After stirred for additional 30 minutes, the suspension was filtrated. The white crystalline precipitate was wash with ^{n}hexane to get pure **4** (46 % yield according to **1**). Colorless block crystals of **4** suitable for X-ray single crystal test were obtained after 1 day from a toluene/ ^{n}hexane solution at -20 °C. ^{1}H NMR (400 MHz, C_6D_6, ppm): δ 7.18-7.17 (m, 3 H, Ar*H*), 7.16-7.14 (m, 5 H, Ar*H*), 7.09-7.06 (m, 4 H, Ar*H*), 6.69 (s, 2 H, Mes*H*), 4.86 (s, 2 H, γ-*H*), 3.69 (sept, *J* = 6.8 Hz, 4 H, C*H*Me$_2$), 3.22 (sept, *J* = 6.8 Hz, 4 H, C*H*Me$_2$), 2.41 (s, 6 H, Mes-*2,6-Me*), 2.10 (s, 3 H, Mes-*4-Me*), 1.56 (s, 6 H, β-*Me*), 1.30 (d, *J* = 6.7 Hz, 12 H, CH*Me$_2$*), 1.23 (d, *J* = 6.8 Hz, 12 H, CH*Me$_2$*), 1.14 (d, *J* = 6.8 Hz, 12 H, CH*Me$_2$*), 1.06 (d, *J* = 6.8 Hz, 12 H, CH*Me$_2$*). ^{13}C{^{1}H} NMR (100 MHz, C_6D_6, ppm): δ 162.92 (*C*N), 145.65,

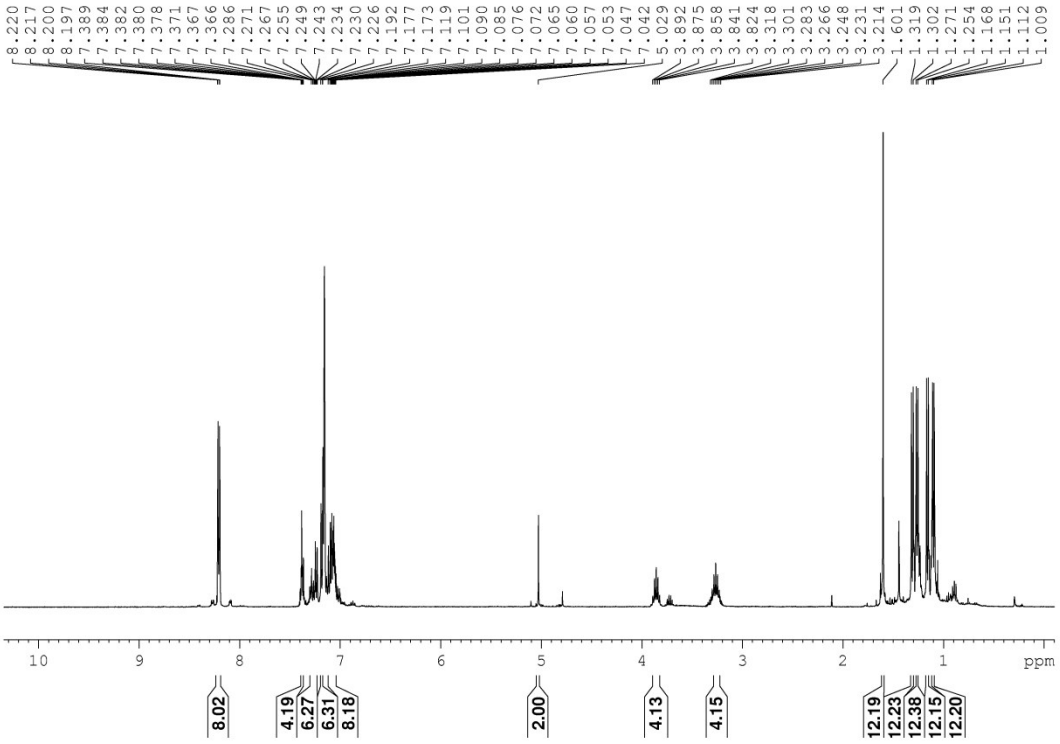
142.58, 140.79, 139.70, 126.50, 123.89, 123.04 (*Ar*), 97.54 (γ-*C*H), 30.91 (Mes-*4-Me*), 28.23, 26.81 (*C*HMe$_2$), 25.94 (β-*Me*), 23.73, 23.64, 23.21, 22.43 (CH*Me$_2$*), 21.99, 21.89 (Mes-*2,6-Me*). ^{11}B NMR (160 MHz, C_6D_6, ppm): δ 18.4 (br, $h_{1/2}$ = 710 Hz), Similar broad ^{11}B signals were reported, see references (N. F. McKinley, D. F. O'Shea, *J. Org. Chem.*, 2004, **69**, 5087-5092; C. Ma, J. Zhang, J. Li, C. Cui, *Chem. Comm.*, 2015, **51**, 5732-5734; and G. Vargas, I. Hernández, H. Höpfl, M.-E. Ochoa, D. Castillo, N. Farfán, R. Santillan, E. Gómez, *Inorg. Chem.*, 2004, **43**, 8490-8500). IR (Nujol mull, cm^{-1}): $\tilde{\nu}$ 2361.4, 1609.5, 1556.4, 1531.0, 1462.4, 1368.4, 1315.3, 1266.3, 1172.3, 1098.8, 1057.9, 1025.5, 857.7, 820.9, 800.5, 759.6, 718.7. ESI-MS: *m/z* = 1215 $[M + H]^+$. Elem. Anal. Calcd for $C_{67}H_{93}B_3Ge_2N_4O_5$: C, 66.39; H, 7.73; N, 4.62; Found: C, 66.68; H, 7.65; N, 4.71.

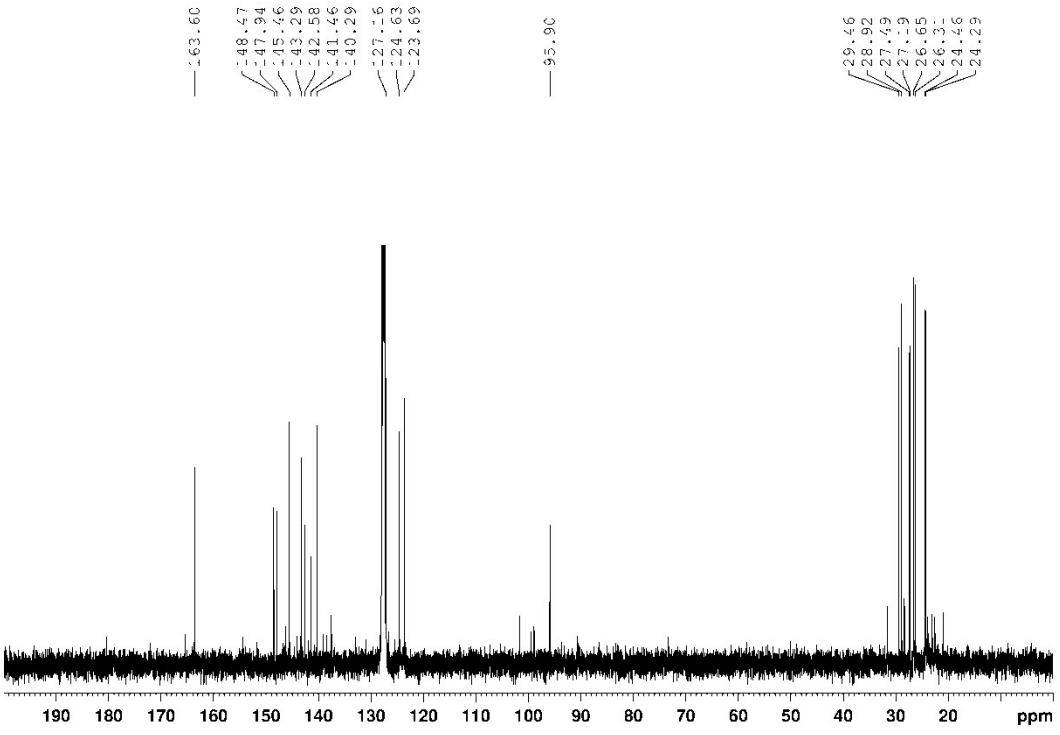
Table S1. Crystal data and structure refinement details for compounds **2**, **3** and **4**

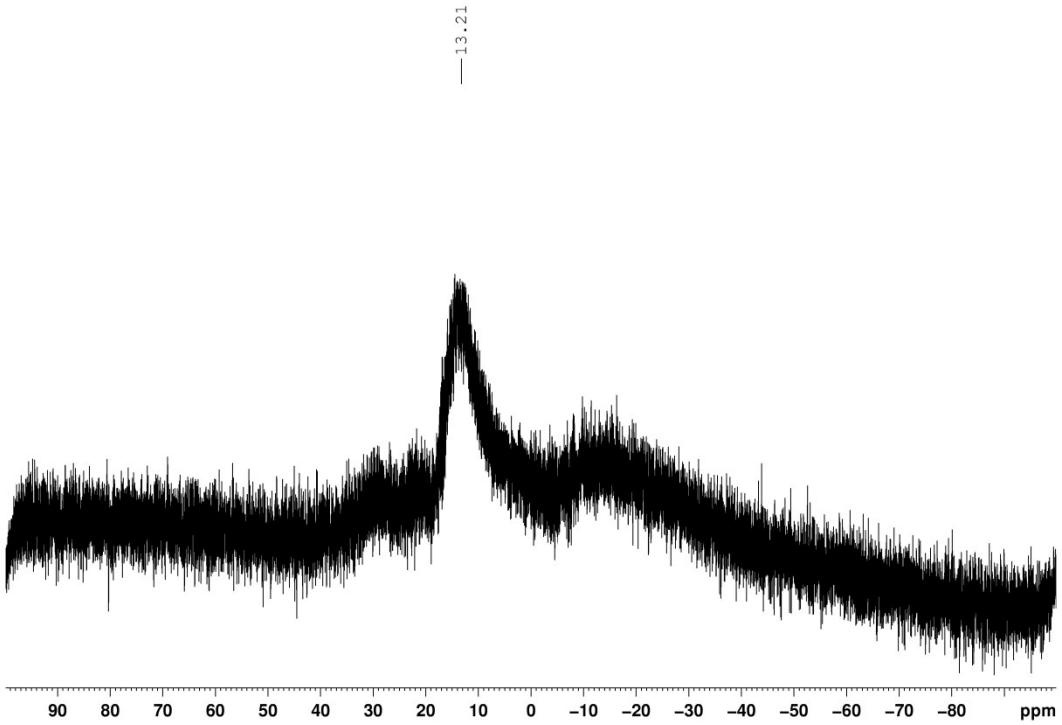
	2·toluene·^{n}hexane	**3**	**4**
CCDC	1027684	1421601	1421455
empirical formula	$C_{95}H_{120}B_4Ge_2N_4O_5$	$C_{41}H_{51}BGeN_2O_2$	$C_{67}H_{95}B_3Ge_2N_4O_5$
formula weight	1590.40	687.24	1214.07
temp, K	173(2)	173(2)	173(2)
cryst syst	triclinic	monoclinic	monoclinic
space group	*P*-1	$P2_1/c$	$P2_1$
a, Å	12.1574(18)	13.605(6)	13.192(8)
b, Å	16.907(3)	14.004(6)	24.045
c, Å	23.516(4)	19.843(11)	13.298
α, deg	110.972(3)	90	90
β, deg	94.490(3)	90.69(4)	93.46(2)
γ, deg	95.764(3)	90	90
V, Å^3	4456.5(12)	3780(3)	4210(3)
Z	2	4	2
D_{calcd}, g/cm^3	1.185	1.208	0.958
μ, mm^{-1}	0.727	0.846	0.864
F(000)	1692.0	1456	0.753
θ range, deg	0.93 -25.01	1.50 - 26.00	1.534 - 28.586
index range	-14 ≤ h ≤ 14	-16 ≤ h ≤ 16	-17 ≤ h ≤ 17
	-19 ≤ k ≤ 20	-17 ≤ k ≤ 17	-32 ≤ k ≤ 31
	-27 ≤ l ≤ 27	-24 ≤ l ≤ 24	-17 ≤ l ≤ 16
reflns collected/unique	32847 / 15618	29129 / 7430	37308 / 19197
	[R(int) = 0.0530]	[*R*(int) = 0.0368]	[R(int) = 0.0754]
data/restraints/param	15618 / 363 / 1026	7430 / 0 / 438	19197 / 221 / 753
GOF on F^2	1.023	1.068	0.921
final R indices	R_1 = 0.0762,	R_1 = 0.0443,	R_1 = 0.0793,
[I >2σ(I)]	wR_2 = 0.2011	wR_2 = 0.1104	wR_2 = 0.1881
R indices (all data)	R_1 = 0.1034,	R_1 = 0.0575,	R_1 = 0.1269,
	wR_2 = 0.2314	wR_2 = 0.1158	wR_2 = 0.2176
largest diff	0.952 / -0.816	0.748 / -0.233	1.04 / -0.41
peak/hole,e/Å^3			

NMR Spectra

2:



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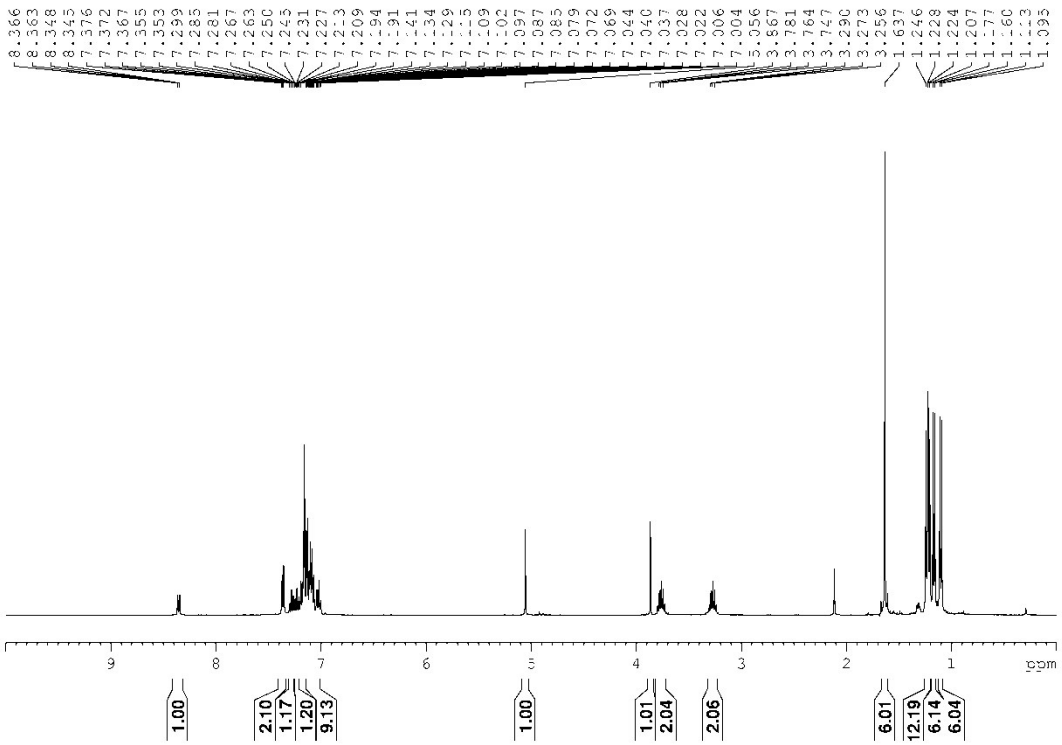
3: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7.079
7.072
7.069
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1.228
1.224
1.207
1.177
1.160
1.143
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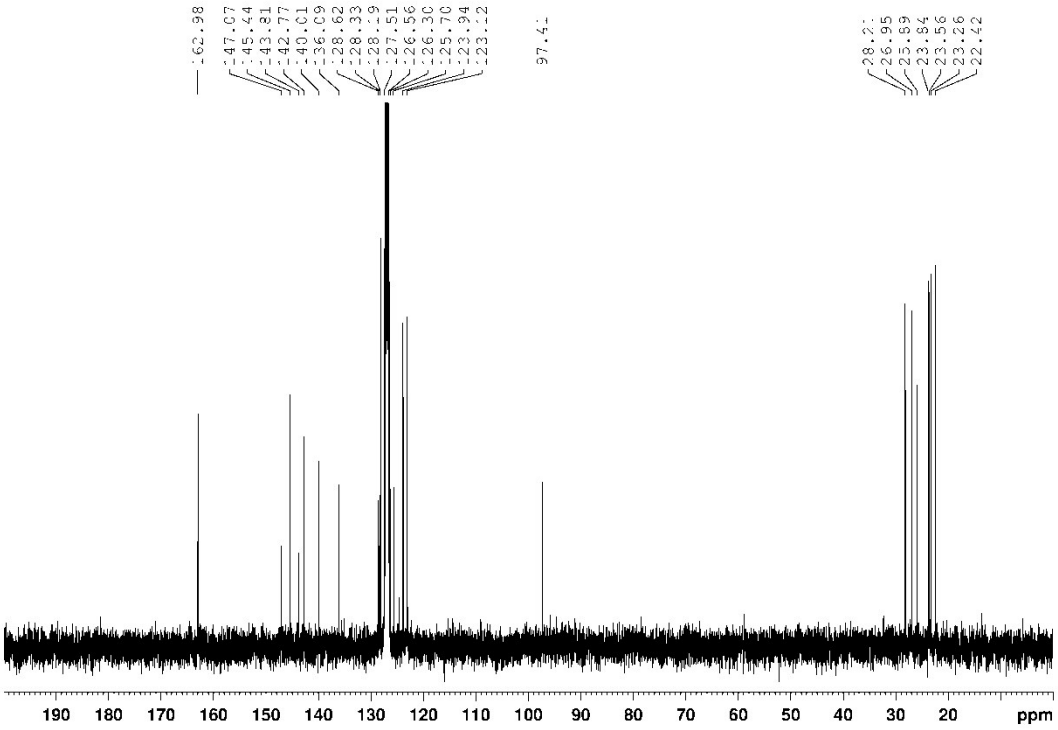
6.04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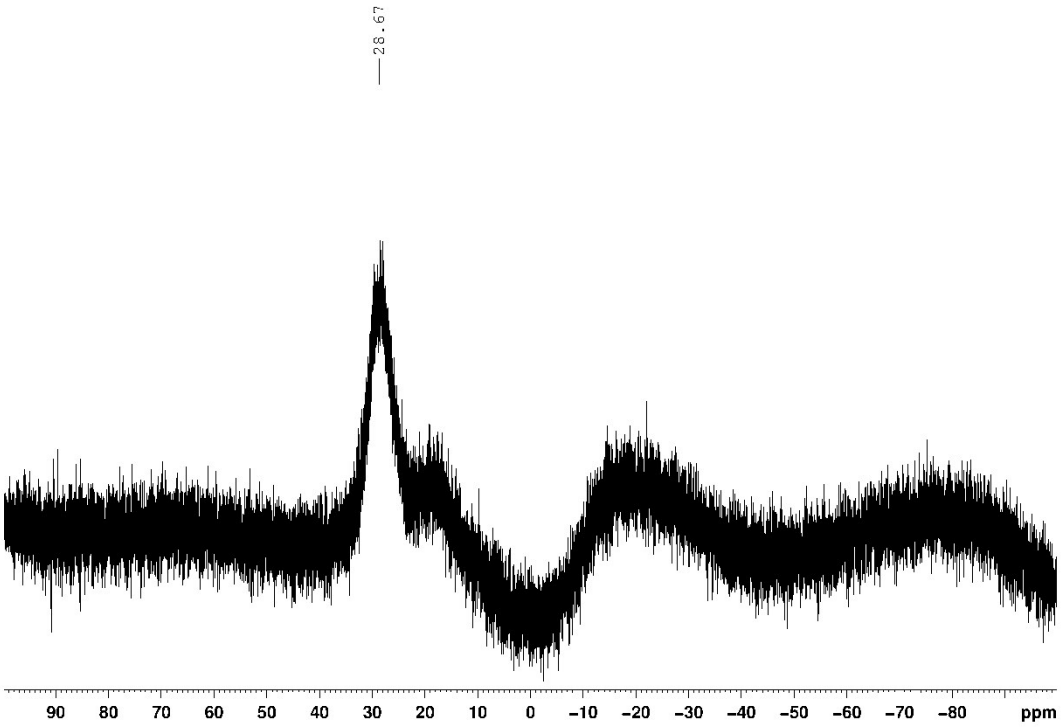
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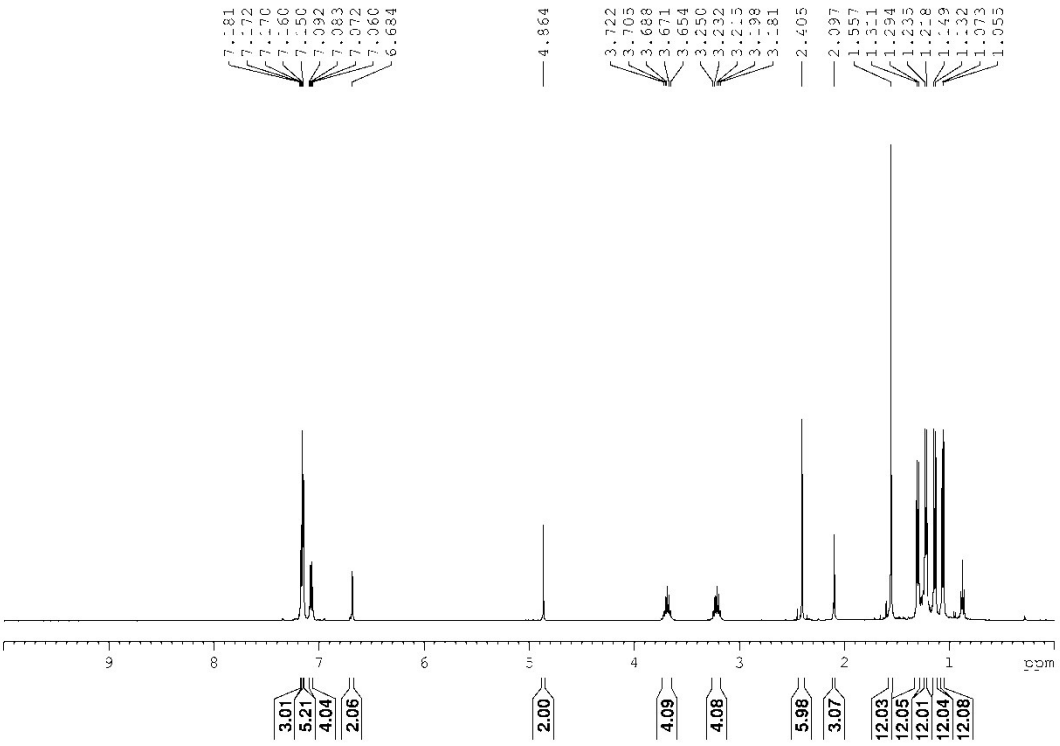
4: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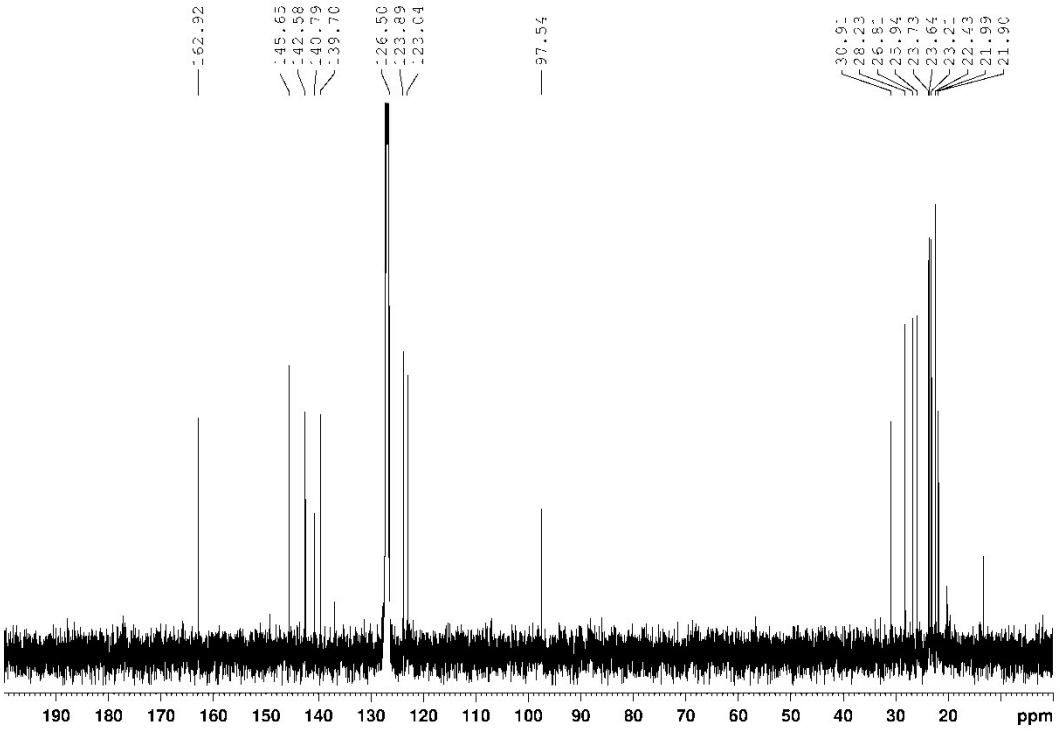
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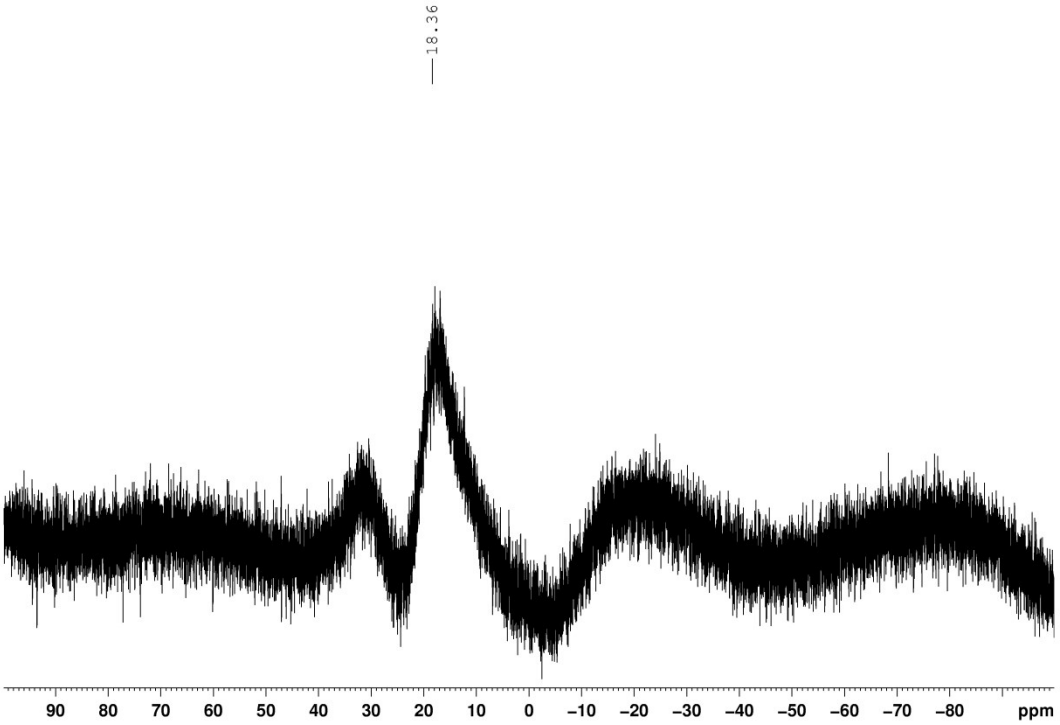
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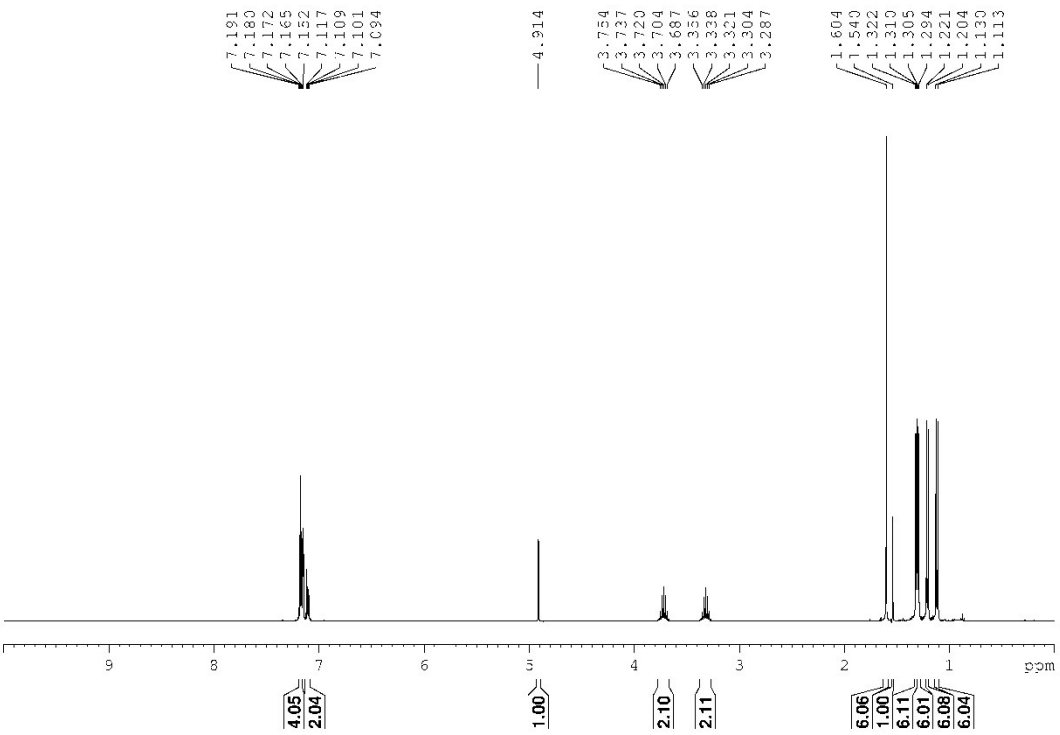
5: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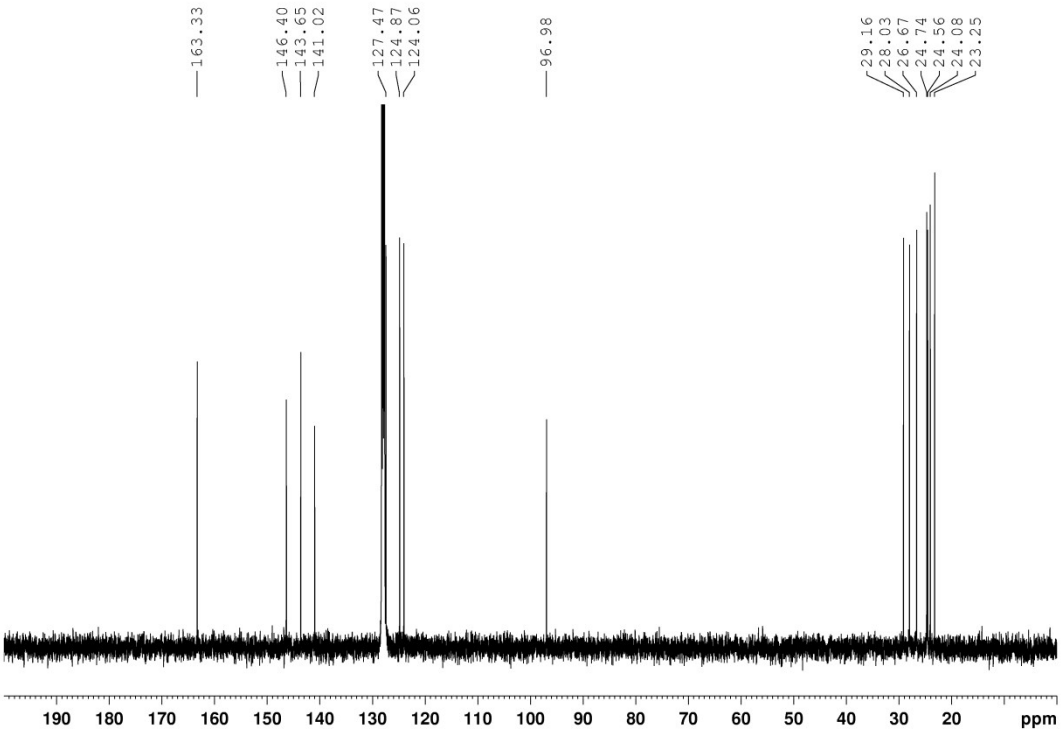
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28.03
26.67
24.74
24.56
24.08
23.25
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

Computational Details

Calculations were performed with the Gaussian 09 package.[s1] Geometry optimizations were carried out with the M06-2X[s2] or B3LYP[s3] functionals and the 6-31G(d) basis set was used for all the atoms. Frequency calculations at the same level of theory were performed to identify the number of imaginary frequencies (zero for local minimum) and provide the thermal corrections of Gibbs free energy and the frontier molecular orbitals (HOMOs and LUMOs).

The M06-2X functional was used for gas-phase, single-point energy calculations. A larger basis set, that is, 6-311++G(2d,p) was used. The Gibbs energy corrections from frequency calculations were added to the single-point energies to obtain the Gibbs free energies. All the free energies reported in the paper correspond to the reference state of 1 mol/L, 298K. Natural bond orbital (NBO) calculations were carried out using NBO 5.9 program[s4] at M06-2X/TZVP[S5]//M06-2X/6-31G(d) level of theory. Optimized structures were visualized by the Chemcraft.[s6]

References:

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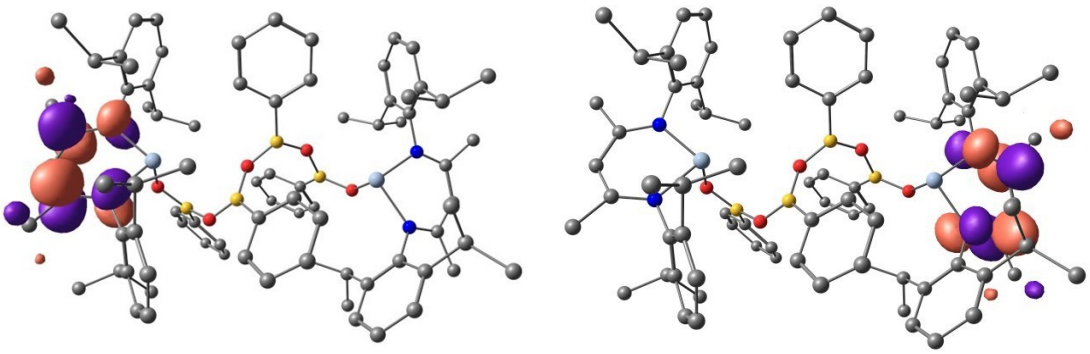

LUMO **LUMO+1**

Fig. S1 LUMO and LUMO+1 of **2**

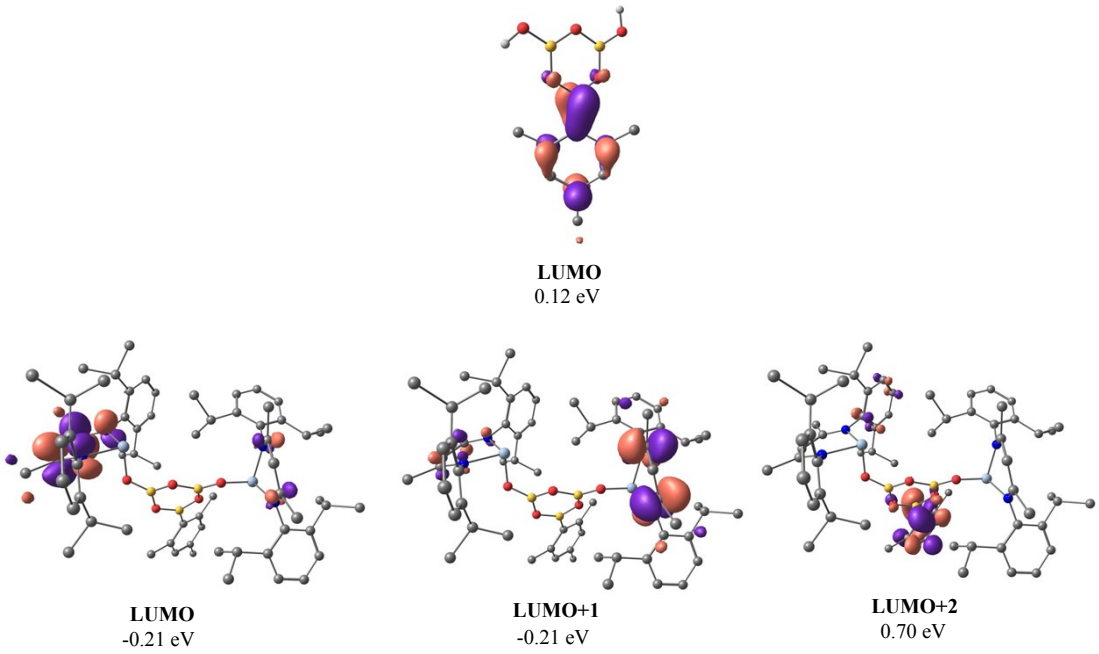

Fig. S2 (top) LUMO of $HOB_2O_3BMesOH$; (bottom) LUMO, LUMO+1 and LUMO+2 of **4**.

Similarly, as shown in Fig. S2, the energy (0.12 eV) of LUMO of $HOB_2O_3BMesOH$ is much lower than that (0.70 eV) of the corresponding LUMO+2 of **4**.

Cartesian coordinates:

2				1	-2.434275	3.195548	2.311270
32	-3.881131	0.027733	-0.272905	1	-3.160136	2.869730	3.896744
32	3.837740	0.164662	-0.370246	1	-3.307841	4.474539	3.170711
7	-5.099212	-1.525817	-0.017150	6	-4.583921	-2.757559	-0.549530
7	-5.428562	1.249124	0.067402	6	-3.691171	-3.532843	0.206665
7	5.378703	1.358706	-0.178614	6	-3.189264	-4.706218	-0.361800
7	5.061446	-1.318310	-0.905071	1	-2.483958	-5.308999	0.204584
8	-3.405454	0.003184	1.546065	6	-3.577005	-5.111321	-1.630468
8	-1.550313	1.283606	0.918919	1	-3.176233	-6.026916	-2.056030
8	0.617276	0.418015	0.505668	6	-4.477496	-4.340767	-2.358708
8	1.842342	-1.535967	0.948683	1	-4.780720	-4.666851	-3.349982
8	3.846476	-0.355803	1.432763	6	-4.995366	-3.156422	-1.835892
5	-2.217776	0.535214	1.885055	6	-3.527627	-4.241666	2.633175
5	-0.378072	1.326973	0.242165	1	-4.576998	-4.555238	2.642066
5	0.911603	-0.882342	0.197689	1	-3.268361	-3.887686	3.636668
5	2.759579	-1.015328	1.871931	1	-2.917011	-5.127410	2.426262
6	-5.082923	2.612603	-0.217323	6	-3.270799	-3.130958	1.609150
6	-5.068250	3.061135	-1.549648	1	-3.851915	-2.250600	1.897733
6	-4.732731	4.394069	-1.793446	6	-1.795139	-2.721121	1.620315
1	-4.722305	4.759267	-2.817691	1	-1.142668	-3.569296	1.375694
6	-4.400851	5.253120	-0.754083	1	-1.514050	-2.328479	2.603631
1	-4.144402	6.287651	-0.962359	1	-1.610250	-1.950560	0.866365
6	-4.372783	4.776769	0.550198	6	-7.728684	1.990426	0.500290
1	-4.083107	5.443258	1.357526	1	-7.353941	2.990620	0.714818
6	-4.689672	3.449657	0.846031	1	-8.511889	1.729645	1.214625
6	-6.425865	2.678394	-3.656632	1	-8.178251	2.017604	-0.500212
1	-7.352071	2.891434	-3.113452	6	-6.642103	0.940654	0.493832
1	-6.646293	1.948035	-4.442408	6	-7.016662	-0.364395	0.850929
1	-6.104548	3.602670	-4.148424	1	-8.007012	-0.491144	1.268131
6	-5.339958	2.134149	-2.722901	6	-6.966467	-2.849664	0.844166
1	-5.696836	1.175650	-2.325486	1	-7.213568	-3.358088	-0.094264
6	-4.031153	1.880549	-3.486237	1	-7.882539	-2.704720	1.417923
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1	-4.207463	1.239099	-4.356750	6	5.002204	2.743461	-0.262772
1	-3.300659	1.395259	-2.829643	6	5.105021	3.386235	-1.511845
6	-5.793289	3.454885	3.130140	6	4.716882	4.722696	-1.598817
1	-5.860540	4.548725	3.097327	1	4.787181	5.239921	-2.552177
1	-5.654798	3.156605	4.174547	6	4.221234	5.398922	-0.488248
1	-6.748802	3.045486	2.791784	1	3.914252	6.436626	-0.576956
6	-4.610735	2.960638	2.285226	6	4.101067	4.739190	0.726386
1	-4.634997	1.867466	2.264071	1	3.690462	5.262855	1.585521
6	-3.298426	3.400877	2.949782	6	4.486802	3.402949	0.862121

6	4.858236	3.421171	3.374788	1	-3.351805	-0.624054	4.090555
1	5.926985	3.621841	3.245129	6	-1.897998	-0.283342	5.648510
1	4.729955	2.824721	4.284387	1	-2.488847	-0.766209	6.422054
1	4.353922	4.379867	3.537374	6	-0.652905	0.261424	5.960380
6	4.277324	2.671012	2.174295	1	-0.266721	0.191870	6.973725
1	4.772955	1.698124	2.101326	6	0.108892	0.875359	4.969387
6	2.778999	2.398487	2.363330	1	1.092785	1.272121	5.206085
1	2.224178	3.332354	2.518257	6	-0.383528	0.953962	3.670662
1	2.615890	1.743089	3.227267	1	0.217892	1.431988	2.900574
1	2.364910	1.900504	1.480857	6	-0.196081	2.469885	-0.806276
6	4.364493	-2.500292	-1.338006	6	-1.326682	3.174798	-1.245437
6	4.281096	-3.590144	-0.448331	1	-2.311057	2.873047	-0.888857
6	3.736926	-4.783923	-0.926179	6	-1.201019	4.222080	-2.152709
1	3.696374	-5.648536	-0.269391	1	-2.085397	4.757558	-2.485696
6	3.228646	-4.877828	-2.216659	6	0.059682	4.583038	-2.624919
1	2.808286	-5.815066	-2.570294	1	0.160386	5.408853	-3.324194
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6	7.138673	-2.409672	-1.631842	1	2.022435	-2.013364	7.189151
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1	7.366255	-1.721043	2.400752
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6	6.517183	0.136757	-0.072340
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1	-7.979096	-0.102155	-2.019984
1	-7.366235	-1.719856	-2.401692
6	5.808966	0.302991	-1.273570
6	1.605433	2.612761	1.475453
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1	3.538040	3.125803	0.691398
6	2.552490	4.862898	1.505864
1	3.370058	5.540651	1.270157
6	1.403420	5.348296	2.135543
1	1.324609	6.403097	2.388954
6	0.355466	4.475791	2.437270
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6	-1.054044	-3.509094	4.643911
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6	0.270503	-1.882281	-2.475017
6	1.002775	-3.067051	-2.266743
1	1.286940	-3.337707	-1.254094
6	1.391821	-3.871518	-3.337666
1	1.958973	-4.781387	-3.156640
6	1.051876	-3.509083	-4.643745
1	1.352306	-4.137361	-5.479097
6	0.330294	-2.335436	-4.874935
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6	-0.051060	-1.532468	-3.799440
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1	2.963922	-0.494713	-2.765566
1	3.650402	1.131972	-2.858957
1	4.494729	-0.246758	-3.613023
6	-4.560247	-1.927948	-2.354632
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1	-3.609522	-2.443085	-2.181332
1	-5.307205	-2.686972	-2.615400
6	-3.901275	0.070147	2.747363
1	-2.964367	-0.493828	2.765232
1	-3.650910	1.132843	2.858568
1	-4.495230	-0.245940	3.612574

2B

8	-1.513705	1.187903	1.986951
8	-2.193268	0.242288	-0.122621
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8	2.542808	-1.625205	-1.690103
5	-2.058922	1.316585	0.743443
5	-1.421497	-0.800983	-0.549369
5	0.884006	-0.975732	0.705828
5	2.881439	-0.654598	-0.785022
6	-2.585230	2.717975	0.297645
6	-2.493367	3.830672	1.154090
1	-2.051729	3.702751	2.138655
6	-2.957628	5.084654	0.759769
1	-2.877774	5.932745	1.435359
6	-3.526915	5.250432	-0.505597
1	-3.889996	6.227527	-0.815244
6	-3.629310	4.159697	-1.371983
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6	-3.162507	2.908349	-0.970461
1	-3.245148	2.061048	-1.646227
6	-2.046833	-1.906103	-1.457684
6	-3.429451	-1.932921	-1.717676
1	-4.063248	-1.163794	-1.283915
6	-3.993626	-2.925407	-2.517753
1	-5.064413	-2.932005	-2.705265
6	-3.178720	-3.911193	-3.080309
1	-3.615570	-4.685632	-3.706186
6	-1.802215	-3.899605	-2.841283
1	-1.167452	-4.663478	-3.283412
6	-1.243978	-2.907273	-2.036237
1	-0.171044	-2.893449	-1.861459
6	0.580481	-1.477259	2.162541
6	-0.627084	-2.123826	2.493010
1	-1.368320	-2.314646	1.719223
6	-0.882646	-2.564558	3.793044
1	-1.817904	-3.068288	4.022173
6	0.068715	-2.362317	4.794392
1	-0.128198	-2.701048	5.808248
6	1.276115	-1.728074	4.489831
1	2.019164	-1.572169	5.267604
6	1.527277	-1.296020	3.188913
1	2.469517	-0.809290	2.953753
6	4.053834	0.365154	-0.997920
6	4.211380	1.452140	-0.118453
1	3.515611	1.564781	0.708355

6	5.235658	2.382286	-0.289891
1	5.334060	3.216501	0.399902
6	6.135807	2.240587	-1.348262
1	6.936769	2.962878	-1.483797
6	6.006394	1.166822	-2.231824
1	6.707299	1.048868	-3.054033
6	4.975493	0.245363	-2.053649
1	4.905473	-0.589101	-2.751543
1	-1.221956	0.288393	2.208275
1	3.066790	-1.580712	-2.501606

NH_3

7	0.000000	0.000000	0.119349
1	0.000000	0.938581	-0.278482
1	-0.812835	-0.469291	-0.278482
1	0.812835	-0.469291	-0.278482

2A-NH_3 adduct (top)

32	-3.098759	-0.643478	-0.132692
32	2.958224	-0.011867	-0.836027
7	-4.215229	0.337264	1.171788
7	-4.564454	-0.597597	-1.467817
7	4.586152	1.191068	-0.778436
7	4.027412	-1.390061	0.223879
8	-2.302000	0.954120	-0.727781
8	-0.331901	-0.032564	-1.679726
8	0.193422	-1.686577	-0.017800
8	0.816538	-0.552554	2.020927
8	2.166787	0.884718	0.537731
5	-1.115180	1.065218	-1.346114
5	0.095911	-1.268531	-1.313659
5	0.172665	-1.524499	1.350731
5	1.490816	0.710684	1.737753
6	-6.560487	0.233313	-2.634322
1	-6.016454	0.516498	-3.543017
1	-7.370055	0.949822	-2.481167
1	-7.008194	-0.750351	-2.821882
6	-5.637416	0.193632	-1.436113
6	-5.971526	0.990775	-0.333454
1	-6.861370	1.599800	-0.430127
6	-5.917549	1.925579	1.976119
1	-6.260159	1.337555	2.836130
1	-6.775840	2.472636	1.580791
1	-5.186469	2.652411	2.347153
6	6.497375	2.354000	0.271620
1	7.170927	2.383694	-0.593245
1	7.113333	2.250122	1.167483
1	5.980975	3.318804	0.319288
6	5.513932	1.202865	0.162724
6	5.668459	0.145371	1.089406
1	6.482148	0.246109	1.797755
6	5.058828	-1.123289	1.016731
6	5.647647	-2.222350	1.879765
1	4.874803	-2.752404	2.447709
1	6.382527	-1.819558	2.580516
1	6.154308	-2.971437	1.258617
6	-5.311421	1.038262	0.907803
6	-0.615618	2.475650	-1.839302
6	-1.389267	3.622185	-1.591295
1	-2.325648	3.506550	-1.052407
6	-0.973916	4.884859	-2.015176
1	-1.588648	5.759024	-1.812097
6	0.234392	5.025905	-2.702413
1	0.561527	6.008097	-3.036498
6	1.018792	3.899213	-2.962920
1	1.954535	4.005302	-3.508227
6	0.593011	2.639083	-2.538317
1	1.209802	1.766606	-2.738707
6	0.496465	-2.284218	-2.449401
6	0.536442	-3.670159	-2.215715
1	0.293633	-4.045059	-1.224135
6	0.872365	-4.569111	-3.230261
1	0.888864	-5.637691	-3.028358
6	1.187608	-4.093413	-4.504505
1	1.452821	-4.789430	-5.296959
6	1.160108	-2.719020	-4.758270
1	1.408896	-2.344819	-5.748687
6	0.816329	-1.829457	-3.741498
1	0.795037	-0.761659	-3.940728
6	-0.568519	-2.642701	2.193998
6	-1.468442	-3.552852	1.608253
1	-1.698520	-3.458443	0.551114
6	-2.099513	-4.539730	2.366467
1	-2.794180	-5.228493	1.891255
6	-1.841102	-4.644073	3.735323
1	-2.329284	-5.415327	4.326627
6	-0.958984	-3.747365	4.342125
1	-0.758895	-3.818347	5.409008

6	-0.339403	-2.758806	3.576525
1	0.338925	-2.055744	4.053971
6	0.651259	1.991509	2.251684
6	-0.143254	1.948379	3.412332
1	-0.242141	1.007078	3.951430
6	-0.819839	3.077169	3.882335
1	-1.425468	3.014607	4.784672
6	-0.719347	4.287254	3.190624
1	-1.245160	5.168960	3.550479
6	0.056840	4.353712	2.031939
1	0.129453	5.286595	1.477538
6	0.732881	3.219315	1.576333
1	1.326911	3.268059	0.668310
6	-4.280108	-1.410218	-2.649481
1	-3.988343	-0.792797	-3.509194
1	-3.441118	-2.076288	-2.422171
1	-5.132621	-2.035279	-2.940496
6	-3.528554	0.420626	2.463043
1	-3.087068	-0.555577	2.690741
1	-2.707581	1.145422	2.407080
1	-4.195555	0.692888	3.283968
6	3.529795	-2.761908	0.110019
1	2.968080	-3.067242	1.003072
1	2.850766	-2.823746	-0.742747
1	4.340111	-3.481903	-0.053144
6	4.479097	2.241375	-1.787892
1	4.306513	1.776989	-2.765486
1	3.610318	2.874780	-1.571074
1	5.370261	2.868541	-1.859713
7	2.813270	0.599750	2.984787
1	2.819721	1.418132	3.592325
1	2.698258	-0.230756	3.564996
1	3.714406	0.545669	2.498473

2A-NH_3 adduct (bottom)

32	-3.232633	-1.170156	0.563084
32	3.333548	-1.060274	-0.620381
7	-4.242585	-0.648308	2.216326
7	-4.838840	-2.141517	-0.116023
7	4.708822	-1.131976	-2.039801
7	4.523961	-2.052803	0.593840
8	-3.697120	0.445523	-0.249378
8	-1.761847	1.462728	-1.308151
8	-0.224595	0.167672	0.049378
8	1.707784	1.507119	0.453135
8	3.894367	0.629320	-0.030684
5	-3.068575	1.459462	-0.878274
5	-0.739246	0.465286	-1.271576
5	0.824897	0.492374	0.817249
5	3.091502	1.635749	0.366316
6	-7.213313	-2.683903	-0.447308
1	-7.219406	-2.358570	-1.494026
1	-8.183385	-2.445006	-0.006512
1	-7.102326	-3.775215	-0.451367
6	-6.090046	-2.022295	0.323375
6	-6.435501	-1.326364	1.491450
1	-7.487583	-1.302863	1.746622
6	-6.164147	-0.084341	3.637095
1	-5.753760	-0.536519	4.548031
1	-7.248380	-0.213196	3.651404
1	-5.945005	0.988939	3.686408
6	6.986326	-0.934189	-2.954484
1	6.922143	-1.722190	-3.715204
1	8.015615	-0.903666	-2.591441
1	6.766721	0.016244	-3.453861
6	6.023164	-1.194753	-1.817387
6	6.565256	-1.535722	-0.571356
1	7.645111	-1.537893	-0.494297
6	5.854441	-2.031620	0.533654
6	6.656029	-2.605484	1.680663
1	6.339597	-2.178875	2.638850
1	7.721571	-2.408164	1.547059
1	6.520499	-3.691878	1.750841
6	-5.558029	-0.705686	2.396467
6	-3.909785	2.770970	-1.179362
6	-5.259346	2.850693	-0.793611
1	-5.701205	1.995148	-0.289098
6	-6.023964	3.989783	-1.047921
1	-7.067218	4.027815	-0.741119
6	-5.448819	5.084451	-1.698565
1	-6.041013	5.974823	-1.898455
6	-4.109183	5.030298	-2.091151
1	-3.656741	5.880668	-2.597269
6	-3.355272	3.884717	-1.832105
1	-2.312228	3.845979	-2.137281
6	-1.006402	-0.866222	-2.155928
6	-0.328158	-2.076605	-1.916399
1	0.381051	-2.138232	-1.095866

6	-0.518723	-3.192889	-2.734521
1	0.017886	-4.116264	-2.525539
6	-1.403680	-3.132346	-3.814538
1	-1.553529	-4.001836	-4.450642
6	-2.090908	-1.944380	-4.071000
1	-2.783313	-1.885059	-4.908220
6	-1.891417	-0.832800	-3.247876
1	-2.439306	0.084770	-3.454061
6	1.045193	-0.272175	2.182145
6	0.348869	-1.468140	2.448585
1	-0.357501	-1.845384	1.713254
6	0.530428	-2.156382	3.649414
1	-0.018021	-3.076999	3.835255
6	1.411974	-1.662389	4.615181
1	1.548727	-2.194735	5.553669
6	2.109793	-0.476465	4.373761
1	2.787786	-0.079779	5.125902
6	1.928641	0.203499	3.167537
1	2.470724	1.131025	2.997970
6	3.710903	3.047745	0.676656
6	2.921624	4.130683	1.102303
1	1.850538	3.987204	1.222728
6	3.486864	5.377439	1.373197
1	2.858538	6.202053	1.701411
6	4.863029	5.564169	1.223217
1	5.307257	6.534281	1.433663
6	5.667992	4.501542	0.803283
1	6.739934	4.645290	0.688109
6	5.094098	3.259630	0.534054
1	5.714886	2.428470	0.209390
6	-4.553052	-2.914601	-1.323794
1	-4.883014	-2.388806	-2.229017
1	-3.471369	-3.055334	-1.408129
1	-5.020970	-3.905912	-1.302211
6	-3.401068	0.050356	3.186358
1	-3.478389	-0.382179	4.191932
1	-2.356585	-0.028954	2.870431
1	-3.648493	1.117980	3.245143
6	3.844314	-2.704579	1.716253
1	3.905425	-2.100334	2.628566
1	2.785539	-2.814290	1.471598
1	4.251423	-3.701400	1.916946
6	4.197285	-0.876704	-3.384441
1	3.137959	-1.153267	-3.413234
1	4.281729	0.185576	-3.653988
1	4.711063	-1.469364	-4.148411
7	0.517884	1.280924	-2.086987
1	1.345174	0.690353	-2.181773
1	0.198157	1.569827	-3.011132
1	0.785641	2.102327	-1.541388

2B-NH_3 adduct (top)

8	0.436261	0.228438	-2.545948
8	1.915279	1.163907	-0.813090
8	0.833349	-0.462208	0.565324
8	-1.182371	-1.677545	0.432499
8	-1.255439	-1.330543	2.752792
5	0.928419	1.368673	-1.856873
5	1.850189	0.433776	0.325662
5	0.132182	-1.512908	0.072900
5	-1.902027	-1.324889	1.544308
6	-0.201680	2.466048	-1.538413
6	-1.461995	2.413349	-2.158224
1	-1.680525	1.585141	-2.828220
6	-2.434815	3.386364	-1.919254
1	-3.404517	3.318363	-2.407652
6	-2.166805	4.443794	-1.047192
1	-2.922979	5.201693	-0.856583
6	-0.924078	4.516533	-0.414657
1	-0.711100	5.330720	0.274600
6	0.041139	3.537814	-0.661519
1	0.999405	3.595881	-0.147093
6	2.946907	0.613263	1.435778
6	4.072899	1.427708	1.220860
1	4.173771	1.943182	0.268828
6	5.053442	1.584097	2.199865
1	5.918129	2.216385	2.012090
6	4.921422	0.927303	3.426093
1	5.682730	1.047885	4.193198
6	3.808123	0.118257	3.665414
1	3.700891	-0.389705	4.620812
6	2.834516	-0.036922	2.678369
1	1.964314	-0.659834	2.869670
6	0.780250	-2.579527	-0.885116
6	-0.024427	-3.526060	-1.546843
1	-1.098626	-3.503200	-1.386578
6	0.529963	-4.482375	-2.396294
1	-0.112278	-5.200851	-2.899494

6	1.912009	-4.518483	-2.599381
1	2.347068	-5.265701	-3.258548
6	2.733417	-3.595921	-1.948590
1	3.810523	-3.627958	-2.092945
6	2.169828	-2.637991	-1.103568
1	2.825732	-1.940730	-0.586483
6	-3.428069	-0.988432	1.391494
6	-3.947226	-0.604673	0.141819
1	-3.277097	-0.549746	-0.711650
6	-5.295696	-0.285814	-0.014213
1	-5.673712	0.016450	-0.987604
6	-6.161158	-0.356367	1.079905
1	-7.213755	-0.112292	0.959628
6	-5.672150	-0.744029	2.329192
1	-6.342973	-0.808216	3.182159
6	-4.319954	-1.051438	2.476974
1	-3.963275	-1.367101	3.457410
1	1.005784	-0.545747	-2.430107
1	-1.823997	-1.018073	3.470130
7	1.956988	2.188581	-3.042024
1	1.433396	2.323766	-3.906772
1	2.262419	3.101564	-2.703416
1	2.786132	1.629410	-3.248803

2B-NH_3 adduct (bottom)

8	-3.920199	0.984171	-2.041559
8	-2.444131	0.931198	-0.232871
8	-0.171863	0.606641	0.603147
8	2.129043	0.880118	0.243120
8	2.413898	-0.214882	2.297584
5	-2.916093	0.323274	-1.360938
5	-1.587232	0.624760	0.879575
5	0.851711	1.410124	0.251930
5	2.744893	-0.102869	0.968448
6	-2.441194	-1.038642	-1.983431
6	-3.192457	-1.608218	-3.030638
1	-4.080346	-1.089914	-3.381285
6	-2.820580	-2.814686	-3.621550
1	-3.420295	-3.234739	-4.425647
6	-1.675676	-3.482243	-3.180255
1	-1.380697	-4.422995	-3.639398
6	-0.910821	-2.935080	-2.148920
1	-0.016049	-3.447263	-1.803633
6	-1.292089	-1.729594	-1.557781
1	-0.680872	-1.319741	-0.760875
6	-2.061071	-0.586819	1.829999
6	-3.412779	-0.962848	1.919737
1	-4.147009	-0.471437	1.283448
6	-3.840558	-1.964598	2.793372
1	-4.892007	-2.239963	2.833197
6	-2.915283	-2.617858	3.609450
1	-3.242127	-3.400595	4.289831
6	-1.566749	-2.262401	3.540782
1	-0.839482	-2.772236	4.169200
6	-1.149006	-1.259880	2.662495
1	-0.094586	-0.998362	2.609383
6	0.739824	2.939202	-0.145062
6	1.836520	3.792411	0.085077
1	2.745994	3.376109	0.509541
6	1.782657	5.151215	-0.224276
1	2.642264	5.787590	-0.028935
6	0.627390	5.692958	-0.792871
1	0.584987	6.750292	-1.042110
6	-0.467811	4.866734	-1.050252
1	-1.361543	5.277378	-1.514060
6	-0.411586	3.508405	-0.726682
1	-1.262821	2.871819	-0.953275
6	3.829667	-1.001686	0.272823
6	4.048563	-0.887627	-1.112424
1	3.463416	-0.167200	-1.676777
6	4.994293	-1.676428	-1.766104
1	5.142718	-1.571748	-2.837797
6	5.750634	-2.601187	-1.042718
1	6.489176	-3.217773	-1.548838
6	5.556920	-2.731782	0.334174
1	6.144618	-3.447949	0.902633
6	4.606864	-1.939140	0.976637
1	4.482944	-2.060239	2.053201
1	-4.154612	1.794197	-1.564854
1	2.889092	-0.933225	2.737395
7	-1.808327	2.020610	1.866518
1	-2.795327	2.126961	2.102036
1	-1.284509	1.924516	2.737357
1	-1.489054	2.866592	1.384708

4

32	-3.345654	-0.519749	-0.036130
32	3.295741	-0.173881	0.332971

8	-1.668314	-0.142589	0.703791	1	-0.585297	-2.184019	0.073795
8	-1.249433	1.590866	-0.876788	6	0.040952	-1.509963	-1.852291
8	0.765516	2.825247	-0.719392	1	0.320049	-1.909657	-2.834434
8	0.498875	0.798035	0.514946	1	0.899632	-0.946161	-1.469983
8	2.667650	1.541957	-0.096399	1	-0.807799	-0.828131	-1.997042
7	-3.005165	-2.453116	0.265525	6	-5.107724	0.655060	1.972007
7	-4.158561	-0.402753	1.764988	6	-4.665999	1.915352	2.411263
7	4.787708	0.598838	1.369811	6	-5.619166	2.911268	2.629100
7	4.449664	-0.206297	-1.290101	1	-5.294158	3.891549	2.967374
6	-2.114979	-4.341679	1.550961	6	-6.969670	2.674899	2.403545
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