Table of Contents

General remarks

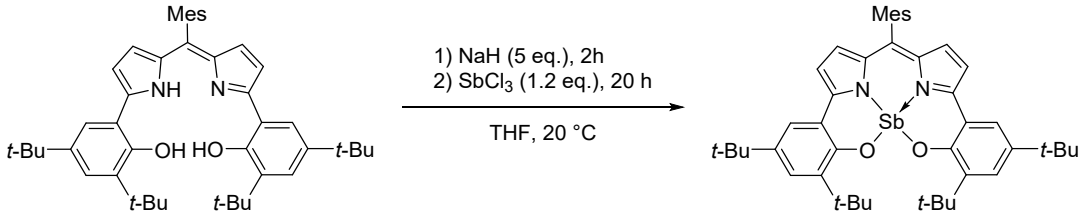
All the manipulations were carried out under dry argon atmosphere using the standard Schlenk technique unless otherwise noted. Ligand **LH_3** was prepared according to a literature.[S1] ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Avance III (^{1}H: 400 MHz, ^{13}C: 100 MHz) or on a JEOL JNM-ECZ600R (^{1}H: 600 MHz, ^{13}C: 150 MHz) spectrometer and referenced to appropriate internal or external standard ($SiMe_4$). Chemical shifts were reported as the delta scale in ppm. High-resolution mass spectra (HRMS) were recorded on a Bruker micrOTOF mass spectrometer (ionization mode: APCI or ESI). UV/vis spectra were recorded on a Shimadzu UV-3101PC or a JASCO V-670 spectrometer. Fluorescence spectra were measured on a Hitachi F-4500 or on a JASCO FP-8600 spectrometer. Photo-luminescence quantum yields (PLQYs) were determined by the absolute method using a JASCO ILF-835 integrating sphere on a JASCO FP-8500 spectrometer (sample concentration: 1.0×10^{-5} M, 293 K).

Author contributions

T. A.: conceptualization, funding acquisition, writing-original draft, and project administration. S. K., R. M., and T. K.: Data curation and investigation, K. K. and H. F. and M. M.: Data curation, supervision, and writing (review and editing), R. I.: Data curation, investigation, validation, visualization, and writing-review and editing, and T. N. conceptualization, funding acquisition, supervision, project administration, and writing-review and editing.

Synthesis of the new compounds

Synthesis of LSb(III)

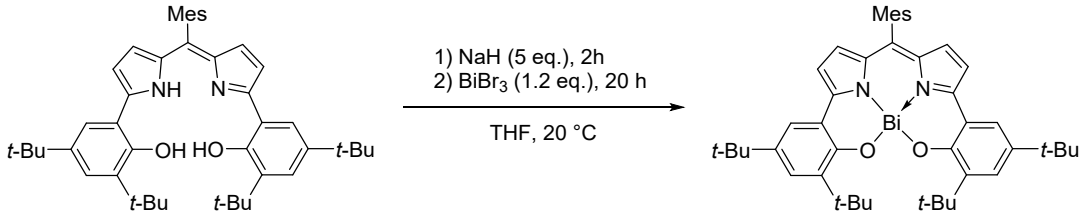


LH_3 **LSb(III)**

To a mixture of NaH (60 wt% dispersion in a mineral oil, 40.5 mg, ca. 1.0 mmol) and THF (1.6 mL) was added **LH_3** (137 mg, 0.20 mmol), and the mixture was stirred at rt for 2 h. $SbCl_3$ (55.2 mg, 0.24 mmol) in THF (10 mL) was added, and the mixture was stirred at rt for 20 h. K_2CO_3 (140 mg, 1.0 mmol) was added, and the mixture was concentrated under reduced pressure. The residue was dissolved in toluene and then stirred at rt for 1 h. The mixture was dissolved in toluene and then filtered using a filter paper. The filtrate was evaporated under reduced pressure. The residue was recrystallized from acetone to afford **LSb(III)** as a dark green solid (72.6 mg, 0.092 mmol, 46%).

^{1}H NMR (acetone-d_6, 400 MHz) δ 7.49 (d, J = 2.4 Hz, 2H), 7.39 (d, J = 2.4 Hz, 2H), 7.01 (d, J = 3.6 Hz, 2H), 6.95 (d, J = 4.6 Hz, 2H), 6.45 (d, J = 4.6 Hz, 2H), 2.35 (s, 3H), 2.21 (s, 3H), 2.17 (s, 3H), 1.55 (s, 18H), 1.32 (s, 18H). ^{13}C NMR (acetone-d_6, 150 MHz) δ 161.65, 156.04, 142.15, 139.98, 139.75, 138.80, 137.48, 137.24, 133.86, 132.47, 128.84, 128.79, 128.04, 127.80, 123.56, 120.37, 118.53, 36.19, 34.77, 31.66, 31.04, 21.18, 20.14, 19.94. HRMS (APCI) m/z calcd for $C_{46}H_{55}N_2O_2{}^{121}Sb$ 789.3374, $C_{46}H_{55}N_2O_2{}^{123}Sb$ 791.3374 ($[M+H]^+$); observed 789.3385.

Synthesis of LBi(III)



LH_3 **LBi(III)**

To a mixture of NaH (60 wt% dispersion in a mineral oil, 44.5 mg, ca. 1.1 mmol) and THF (1.6 mL) was added **LH_3** (151 mg, 0.22 mmol), and the mixture was stirred at rt for 2 h. $BiBr_3$ (120 mg, 0.27 mmol) in THF (10 mL) was added, and the mixture was stirred at rt for 20 h. K_2CO_3 (154 mg, 1.1 mmol) was added, and the mixture was concentrated under reduced pressure. The residue was dissolved in toluene and then stirred at rt for 1 h. The mixture was dissolved in AcOEt

and filtered using a filter paper. The filtrate was evaporated under reduced pressure. The residue was dissolved in hexane and then stirred at rt for 1 h. The mixture was filtered using a filter paper and concentrated in vacuo to afford **LBi(III)** as a dark green solid (76.1 mg, 0.087 mmol, 39%).

^{1}H NMR (acetone-$\boldsymbol{d}_6$, 400 MHz) δ 7.41 (d, J = 2.4 Hz, 2H), 7.37 (d, J = 2.4 Hz, 2H), 6.98-6.95 (m, 4H), 6.41 (d, J = 4.4 Hz, 2H), 2.34 (s, 3H), 2.22 (s, 3H), 2.15 (s, 3H), 1.54 (s, 18H), 1.30 (s, 18H). ^{13}C NMR (acetone-d_6, 150 MHz) δ 162.85, 157.71, 143.02, 140.96, 140.35, 139.36, 138.18, 137.31, 137.28, 135.47, 132.23, 128.66, 128,53, 126.60, 123.37, 122.84, 118.02, 36.16, 34.47, 31.98, 31.04, 21.18, 20.23, 20.00. HRMS (APCI) m/z calcd for $C_{46}H_{55}N_2O_2Bi$ 877.4140 ($[M+H]^+$); observed 877.4048.

Crystallographic analysis

Single crystal X-ray diffraction (XRD) measurements were carried out on a Rigaku MicroMax-007HF diffractometer equipped with a VariMax light source (Mo Kα, λ = 0.71073 Å). The crystals were kept at –60 °C while the data collection. The collected data were processed using the CrysAlisPro (ver. 1.171.41.117a) program package (Rigaku Oxford Diffraction, 2021). Using Olex2,[S2] the structures were solved with the SHELXT and refined with the SHELXL program packages.[S3] The full-matrix least-squares refinements were performed on F^2. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. Crystallographic data are summarized in the next page. CCDC 2421517 (**LSb(III)**) and 2421518 (**LBi(III)**) contain additional crystallographic data.

Table S1. Crystallographic data.

	LSb(III)	**LBr(III)**-CH_2Cl_2
Empirical formula	$C_{46}H_{55}N_2O_2Sb$	$C_{47}H_{57}N_2O_2Cl_2Bi$
Formula weight	789.67	961.82
Crystal system	orthorhombic	triclinic
Space group	*P*bca	*P*-1
a/Å	18.4576(6)	13.8968(10)
b/Å	16.2320(6)	14.1548(10)
c/Å	27.3781(10)	14.2678(10)
β/°	90	80.924(6)
V/Å^3	8202.6(5)	2197.8(3)
Z	8	2
ρ/g cm^{-3}	1.279	1.453
μ/mm^{-1}	0.711	4.171
F(000)	3296.0	972.0
Crystal size/mm^3	0.1 × 0.1 × 0.02	0.2 × 0.2 × 0.1
2Θ/°	4.410 to 55.810	4.440 to 55.614
Index ranges	$-24 \le h \le 24$, $-20 \le k \le 20$, $-21 \le l \le 32$	$-16 \le h \le 16$, $-14 \le k \le 18$, $0 \le l \le 18$
Reflections collected	34983	8844
Independent reflections (R_{int}, R_σ)	8641 (0.1111, 0.0912)	9643 (0.0352, 0.0170)
Data/restraints/parameters	8597/4/485	8844/472/506
GOF on F^2	1.025	1.104
R_1 ($I \ge 2\sigma$ (I))	0.0482	0.0991
Empirical formula	$C_{46}H_{55}N_2O_2Sb$	$C_{47}H_{57}N_2O_2Cl_2Bi$
Formula weight	789.67	961.82
Crystal system	orthorhombic	triclinic
CCDC No.	2421517	2421518

DFT calculations

Density functional theory (DFT) calculations were performed using the Gaussian 16 (revision C.02) program package.[S4] B3LYP density functional with the GD3BJ empirical dispersion correction were employed to the geometry optimizations and the time-dependent (TD)-DFT calculations. The 6-31g(d) basis set for H, C, N, and O atoms and LanL2DZ basis set for the Sb and Bi atoms were used. The optimized geometries were confirmed as the local energy minima by the frequency calculations. The computation was performed using Research Center for Computational Science, Okazaki, Japan (Project: 23-IMS-C170 and 24-IMS-C172, T.A.).

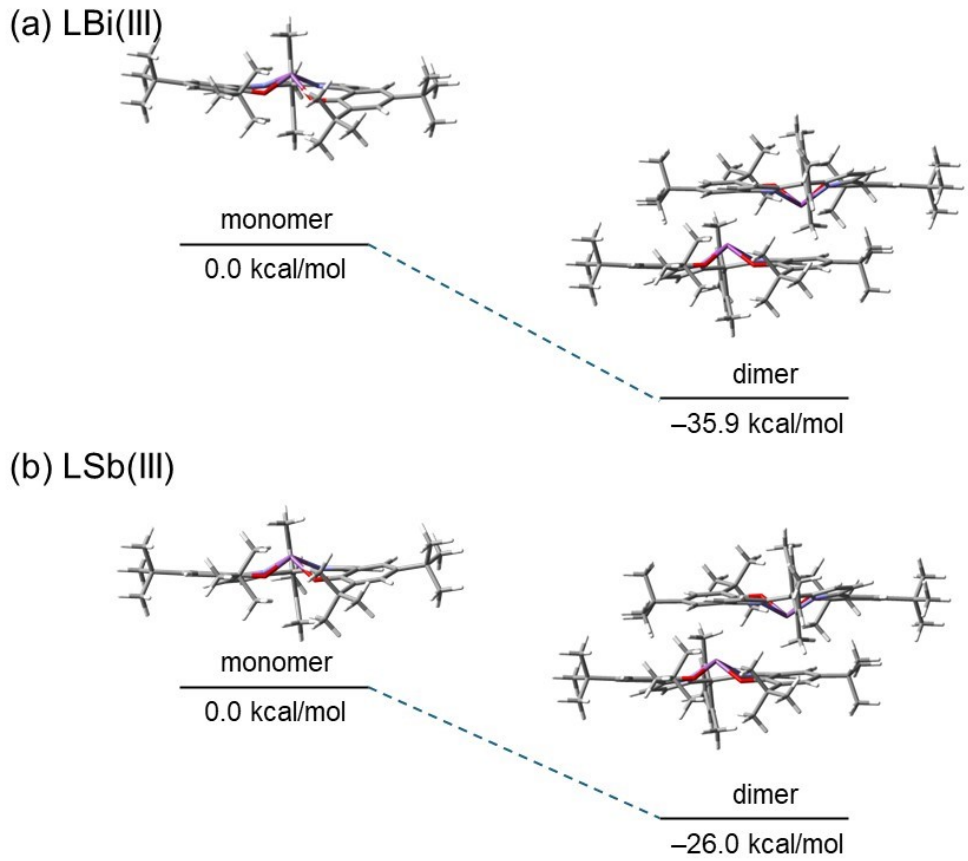
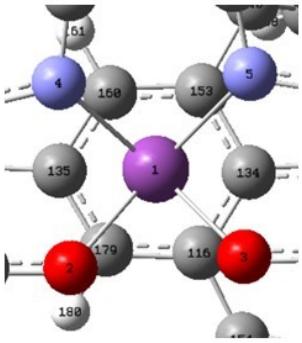


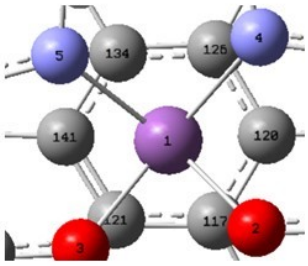
Figure S1. Dimerization energy estimated by relative Gibbs free energy at 298 K for (a) **LBi(III)** and (b) **LSb(III)** (B3LYP-GD3BJ/6-31g(d), LanL2DZ).

(a) Lbi(III)-dimer



Donor	Acceptor	kcal/mol
BD (1) C116- C134	LV (1)Bi 1	0.41
BD (2) C116- C134	LV (1)Bi 1	3.61
BD (2) C116- C134	LV (2)Bi 1	1.48
BD (2) C116- C134	LV (3)Bi 1	0.38
BD (1) C116- C179	LV (1)Bi 1	0.31
BD (1) C134- C153	LV (1)Bi 1	0.24
BD (1) C135- C160	LV (1)Bi 1	0.16
BD (1) C135- C160	LV (2)Bi 1	0.05
BD (1) C135- C179	LV (1)Bi 1	0.24
BD (1) C135- C179	LV (2)Bi 1	0.07
BD (2) C135- C179	LV (1)Bi 1	2.11
BD (2) C135- C179	LV (2)Bi 1	3.14
BD (2) C135- C179	LV (3)Bi 1	0.08
BD (1) C153- C160	LV (1)Bi 1	0.13
BD (1) C153- C160	LV (3)Bi 1	0.07
BD (2) C153- C160	LV (1)Bi 1	0.72
BD (2) C153- C160	LV (3)Bi 1	2.85

(b) LSb(III)-dimer



Donor	Acceptor	kcal/mol
BD (1) C117- C120	LV (1)Sb 1	0.12
BD (2) C117- C120	LV (1)Sb 1	1.84
BD (2) C117- C120	LV (2)Sb 1	0.67
BD (2) C117- C120	LV (3)Sb 1	0.31
BD (1) C117- C121	LV (1)Sb 1	0.08
BD (1) C120- C126	LV (1)Sb 1	0.06
BD (1) C121- C141	LV (1)Sb 1	0.05
BD (1) C121- C141	RY (2)Sb 1	0.08
BD (2) C121- C141	LV (1)Sb 1	0.89
BD (2) C121- C141	LV (2)Sb 1	1.86
BD (1) C126- C134	RY (1)Sb 1	0.08
BD (2) C126- C134	LV (1)Sb 1	0.33
BD (2) C126- C134	LV (3)Sb 1	1.18

Figure S2. The second-order perturbation interaction energies between (a) Bi-dimer and (b) Sb-dimer calculated by NBO analysis (B3LYP-GD3BJ/6-31g(d), LanL2DZ).

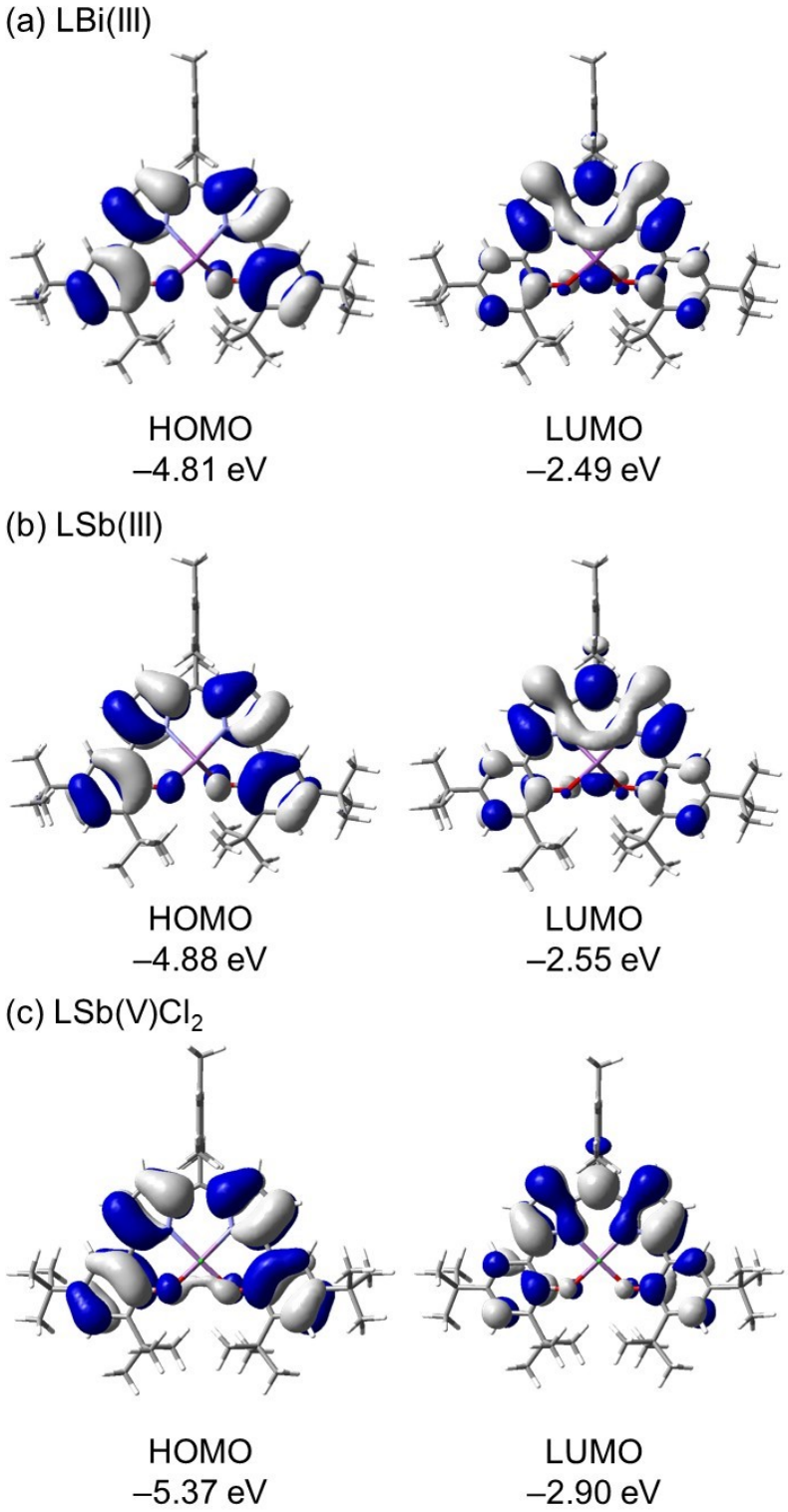
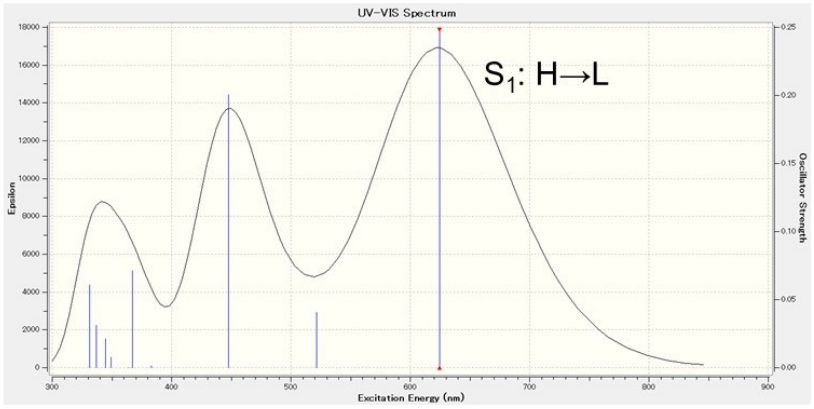
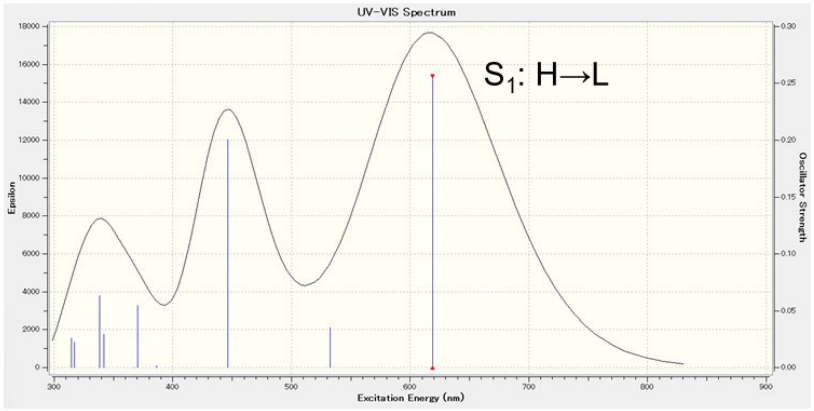


Figure S3. Frontier orbitals of (a) **LBi(III)**, (b) **LSb(III)**, and (c) **LSb(V)Cl_2** (B3LYP-GD3BJ/6-31g(d), LanL2DZ).

(a) LBi(III)



(b) LSb(III)



(C) $LSb(V)Cl_2$

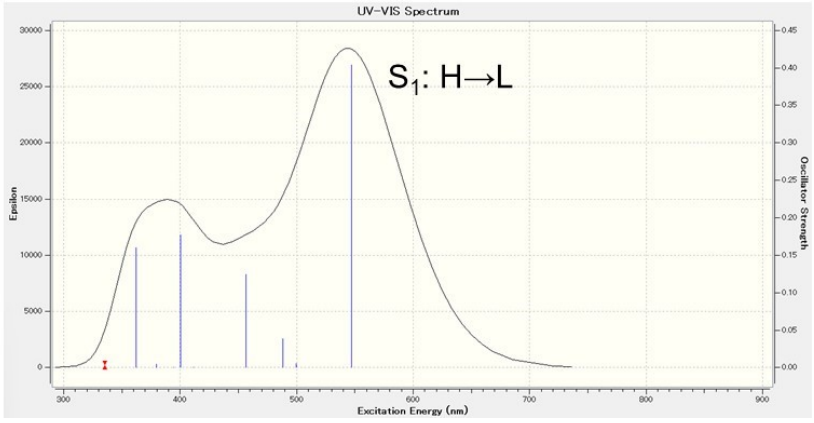


Figure S4. Calculated UV-vis spectrum of (a) **LBi(III)**, (b) **LSb(III)**, and (c) **$LSb(V)Cl_2$** simulated by TD-DFT calculation (TD-B3LYP-GD3BJ/6-31G(d), LanL2DZ//B3LYP-GD3BJ/6-31G(d), LanL2DZ).

Table S2. Cartesian coordinates of **LBi(III)-monomer** in the S_0 state.

atom	x	y	z
Bi	-0.032628	-0.274283	-0.833155
O	1.323403	-1.573443	0.139139
O	-1.314832	-1.411301	0.401649
N	1.404821	1.245389	-0.011386
N	-1.484408	1.302323	-0.101845
C	2.451838	3.227909	0.412102
H	2.596603	4.28262	0.59889
C	0.111307	6.96327	-0.831509
H	0.191511	7.57204	-1.72948
C	-3.413764	-0.27263	-0.019857
C	1.196616	2.624891	0.129435
C	0.09829	5.571657	-0.957516
C	-0.106804	5.389906	1.471038
C	5.515054	-1.512124	0.040948
C	2.737978	0.993558	0.172722
C	3.398234	2.225611	0.454984
H	4.444534	2.339823	0.694571
C	4.794868	-0.332727	0.037091
H	5.315607	0.612533	-0.023402
C	-0.088309	6.785238	1.552578
H	-0.164047	7.254633	2.530976
C	-0.011089	4.785416	0.203641
C	7.046232	-1.56581	-0.017979
C	3.382078	-0.309329	0.090714
C	2.656033	-4.116901	0.140379
C	4.776081	-2.708467	0.098388
H	5.325624	-3.640486	0.10218
C	-2.656788	-1.436619	0.27978
C	-5.484907	-1.571595	-0.064132
C	3.386821	-2.764397	0.129344
C	0.022925	7.589167	0.414801
C	-2.562658	3.300722	0.106876
H	-2.721661	4.363263	0.227468
C	-2.579565	-3.934323	0.924557
C	1.859125	-4.268322	-1.174608
H	2.541163	-4.267761	-2.033132
H	1.304279	-5.213661	-1.180064
H	1.144426	-3.455355	-1.300367
C	-3.511747	2.298731	0.10384
H	-4.578029	2.415801	0.230475
C	-0.034871	3.292571	0.084115
C	-0.230164	4.552175	2.721191
H	-0.257986	5.184044	3.613533
H	-1.14136	3.943686	2.704401
H	0.611595	3.857636	2.819084
C	2.664033	-1.533237	0.11242
C	-3.340229	-2.668442	0.498403
C	-2.819979	1.0547	-0.029128
C	7.48576	-2.344121	-1.277347
H	8.579775	-2.400815	-1.33177
H	7.097381	-3.367746	-1.275994
H	7.122305	-1.849541	-2.18506
C	-1.285973	2.678257	-0.009097
C	-4.719725	-2.691254	0.312861
H	-5.237806	-3.630344	0.455819
C	0.194789	4.924434	-2.31819
H	1.080007	4.281629	-2.388714
H	-0.677136	4.290652	-2.51783
H	0.256901	5.678274	-3.108256
C	-3.520308	-5.131633	1.151808
H	-4.049519	-5.421879	0.236729
H	-2.927211	-5.993648	1.475961
H	-4.262991	-4.929158	1.931876
C	-1.578469	-4.335473	-0.178263
H	-0.836743	-3.554875	-0.331432
H	-1.051651	-5.254311	0.103614
H	-2.101593	-4.521002	-1.124299
C	-6.995947	-1.719919	-0.277723
C	3.629685	-5.307759	0.21874

H	4.243179	-5.275445	1.126252
H	3.052344	-6.23845	0.242591
H	4.297183	-5.35777	-0.649109
C	-4.809454	-0.373494	-0.209481
H	-5.347688	0.524339	-0.483623
C	-7.656892	-0.392777	-0.684594
H	-7.531823	0.374725	0.087545
H	-7.244075	-0.006298	-1.623244
H	-8.732031	-0.543955	-0.831185
C	1.724333	-4.208487	1.368095
H	0.990914	-3.404715	1.373114
H	1.193415	-5.167921	1.366418
H	2.311749	-4.149578	2.292089
C	7.674516	-0.163809	-0.075604
H	7.352957	0.387801	-0.966242
H	7.417585	0.430699	0.808411
H	8.766157	-0.248422	-0.113454
C	-7.654656	-2.205826	1.031814
H	-8.736638	-2.323769	0.896177
H	-7.250881	-3.170941	1.35423
H	-7.486176	-1.486011	1.84042
C	-1.839634	-3.667716	2.254927
H	-2.55955	-3.438714	3.049585
H	-1.273373	-4.557168	2.555512
H	-1.147485	-2.830665	2.161347
C	0.072962	9.093298	0.53165
H	-0.328221	9.577775	-0.364647
H	-0.499755	9.446716	1.395486
H	1.10496	9.446303	0.658817
C	7.582037	-2.283333	1.240209
H	8.677103	-2.339258	1.213065
H	7.287852	-1.745054	2.147995
H	7.196781	-3.305093	1.318197
C	-7.257056	-2.752396	-1.39604
H	-6.805781	-2.424759	-2.339269
H	-6.837203	-3.732407	-1.147268
H	-8.334441	-2.880126	-1.557064

Table S3. Cartesian coordinates of **LBi(III)-dimer** in the S_0 state.

atom	x	y	z
Bi	-2.349006	0.082038	0.339918
O	-3.312956	-1.534036	1.346746
O	-1.03434	-0.350607	1.971918
N	-4.40031	0.973085	0.657776
N	-1.796032	2.164962	1.113728
C	-6.179439	2.39814	0.53806
H	-6.74646	3.317936	0.511179
C	-5.184312	6.671896	-0.791185
H	-5.28311	7.146812	-1.764865
C	0.47586	1.544233	1.946171
C	-4.75841	2.324816	0.590124
C	-4.61865	5.395994	-0.716716
C	-4.914815	5.445933	1.70799
C	-7.033379	-3.192605	0.353057
C	-5.542708	0.226987	0.647058
C	-6.665126	1.108732	0.587344
H	-7.702611	0.810775	0.614411
C	-6.835335	-1.825737	0.30443
H	-7.626427	-1.179453	-0.049725
C	-5.475106	6.72071	1.589124
H	-5.804321	7.234886	2.489469
C	-4.487195	4.782931	0.541543
C	-8.338748	-3.870979	-0.077483
C	-5.608905	-1.227653	0.671035
C	-3.583158	-4.393848	1.62463
C	-5.957893	-3.974168	0.81379
H	-6.102386	-5.044793	0.872037
C	0.148061	0.191351	2.257852
C	2.747314	1.248181	2.837428
C	-4.715141	-3.458728	1.16809
C	-5.622077	7.349424	0.349441
C	-1.621088	4.441568	1.102972
H	-1.898408	5.483431	1.025282
C	0.770691	-2.029145	3.418209
C	-2.437692	-4.357742	0.591269
H	-2.788645	-4.738781	-0.375338
H	-1.601235	-4.984602	0.919866
H	-2.064645	-3.345033	0.450015
C	-0.400377	3.919626	1.480009
H	0.479413	4.47896	1.759376
C	-3.8827	3.415575	0.649362
C	-4.770578	4.798874	3.064561
H	-5.169064	5.447028	3.850331
H	-3.720198	4.587792	3.294758
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C	-4.515426	-2.046924	1.060853
C	1.118741	-0.61248	2.937991
C	-0.530049	2.496489	1.488991
C	-8.048492	-4.843418	-1.24168
H	-8.967858	-5.351115	-1.558043
H	-7.322172	-5.611125	-0.956083
H	-7.641114	-4.303206	-2.103598
C	-2.50419	3.344268	0.888675
C	2.372622	-0.063094	3.192208
H	3.101644	-0.673319	3.706091
C	-4.136928	4.698151	-1.964077
H	-4.574508	3.697456	-2.053928
H	-3.049231	4.56954	-1.94859
H	-4.396364	5.266812	-2.86172
C	1.936258	-2.685842	4.179435
H	2.832221	-2.788096	3.559113
H	1.635607	-3.691918	4.490998
H	2.20348	-2.126334	5.083091
C	0.434136	-2.927058	2.210575
H	-0.416409	-2.537137	1.656531
H	0.185049	-3.939291	2.548664
H	1.289812	-3.00156	1.530766
C	4.123178	1.785047	3.255849

C	-4.043528	-5.858457	1.742766	H	5.116562	-0.170556	3.472246
H	-4.863627	-5.973624	2.460488	H	6.212814	1.183528	3.189268
H	-3.204578	-6.467314	2.097254	Bi	2.349039	-0.082184	-0.339733
H	-4.365036	-6.272219	0.780037	O	3.312074	1.534433	-1.3467
C	1.777418	2.02897	2.223531	O	1.033793	0.350097	-1.971268
H	2.007384	3.048225	1.94967	N	4.400463	-0.972522	-0.658641
C	4.461665	3.114166	2.562575	N	1.796339	-2.165242	-1.113322
H	3.759425	3.908448	2.839425	C	6.180069	-2.397117	-0.54061
H	4.462952	3.017413	1.47463	H	6.747348	-3.316773	-0.514395
H	5.460734	3.444114	2.865871	C	5.190266	-6.668991	0.791825
C	-3.072885	-3.957756	3.013446	H	5.292164	-7.142411	1.765901
H	-2.710985	-2.932194	2.993049	C	-0.475821	-1.545248	-1.945427
H	-2.254584	-4.612564	3.336504	C	4.758965	-2.324163	-0.591395
H	-3.877617	-4.030596	3.754658	C	4.62405	-5.393284	0.717144
C	-9.390197	-2.855159	-0.552783	C	4.912861	-5.446888	-1.708369
H	-9.036756	-2.283015	-1.418115	C	7.032384	3.193811	-0.353941
H	-9.657141	-2.148013	0.240648	C	5.542656	-0.22612	-0.64869
H	-10.30416	-3.379993	-0.851909	C	6.665364	-1.107571	-0.590079
C	4.098437	2.016107	4.784037	H	7.702734	-0.809291	-0.617983
H	5.06867	2.392793	5.130243	C	6.834813	1.826851	-0.305843
H	3.882185	1.087249	5.323173	H	7.626251	1.180661	0.047711
H	3.329056	2.747824	5.054279	C	5.473866	-6.721267	-1.589285
C	-0.424953	-1.946618	4.394076	H	5.800628	-7.236646	-2.489847
H	-0.154299	-1.34764	5.271654	C	4.488499	-4.782253	-0.54159
H	-0.697908	-2.950385	4.738729	C	8.337701	3.872433	0.07636
H	-1.294049	-1.493794	3.917868	C	5.608417	1.228545	-0.672171
C	-6.261284	8.712822	0.244297	C	3.581299	4.394447	-1.623776
H	-5.895032	9.25996	-0.630579	C	5.956455	3.975215	-0.813899
H	-6.060012	9.318656	1.134093	H	6.100583	5.045911	-0.87175
H	-7.35197	8.632161	0.145668	C	-0.148371	-0.192326	-2.257314
C	-8.928493	-4.65801	1.112826	C	-2.747161	-1.250053	-2.837287
H	-9.859413	-5.158125	0.819115	C	4.713726	3.459525	-1.167935
H	-9.148612	-3.986554	1.950116	C	5.6247	-7.348119	-0.349052
H	-8.236026	-5.425561	1.473268	C	1.621695	-4.441851	-1.100997
C	5.234474	0.768153	2.921668	H	1.899129	-5.483638	-1.022676
H	5.253133	0.537842	1.854691	C	-0.77165	2.028032	-3.417633

C	2.436083	4.357482	-0.590181	H	3.201829	6.467987	-2.09538
H	2.787126	4.738178	0.376531	H	4.362762	6.272729	-0.778606
H	1.599344	4.984227	-0.918281	C	-1.777185	-2.030404	-2.222958
H	2.063393	3.344588	-0.449324	H	-2.00689	-3.049699	-1.949027
C	0.400755	-3.920309	-1.477885	C	-4.46109	-3.116407	-2.562415
H	-0.479088	-4.479971	-1.756433	H	-3.758461	-3.910622	-2.838463
C	3.883486	-3.415156	-0.649565	H	-4.462997	-3.019075	-1.474527
C	4.764398	-4.801853	-3.065451	H	-5.45989	-3.44682	-2.866088
H	5.164099	-5.449452	-3.851061	C	3.070846	3.958733	-3.012645
H	3.71293	-4.594846	-3.294425	H	2.709397	2.933005	-2.992578
H	5.292349	-3.842783	-3.110353	H	2.252175	4.613324	-3.335203
C	4.514484	2.047617	-1.061163	H	3.875348	4.032228	-3.754042
C	-1.119201	0.611159	-2.937631	C	9.38961	2.85678	0.551003
C	0.530251	-2.497155	-1.487874	H	9.036615	2.28426	1.416268
C	8.047576	4.844448	1.240939	H	9.656517	2.149962	-0.242732
H	8.966918	5.352277	1.557158	H	10.30351	3.381797	0.849997
H	7.320978	5.612066	0.955812	C	-4.096954	-2.019385	-4.784244
H	7.640606	4.303879	2.102829	H	-5.066888	-2.396511	-5.130811
C	2.504766	-3.344303	-0.887861	H	-3.88064	-1.090744	-5.323728
C	-2.372813	0.061291	-3.192156	H	-3.32722	-2.751033	-5.053667
H	-3.101887	0.67116	-3.706378	C	0.424027	1.946125	-4.393488
C	4.146387	-4.693449	1.964966	H	0.153656	1.347117	-5.271132
H	4.587684	-3.694296	2.054123	H	0.696564	2.950041	-4.738041
H	3.059172	-4.560933	1.950738	H	1.293313	1.493624	-3.917307
H	4.404873	-5.262893	2.862381	C	6.264454	-8.711279	-0.244152
C	-1.937502	2.684395	-4.178727	H	5.912716	-9.251173	0.641068
H	-2.833745	2.785588	-3.558626	H	6.047474	-9.323893	-1.125632
H	-1.637501	3.690855	-4.489661	H	7.356751	-8.630952	-0.165098
H	-2.204099	2.125183	-5.082759	C	8.926794	4.659981	-1.113934
C	-0.435419	2.925881	-2.209839	H	9.857676	5.160283	-0.820422
H	0.4154	2.536312	-1.655978	H	9.146797	3.988831	-1.951499
H	-0.186886	3.938307	-2.547777	H	8.233963	5.427431	-1.473897
H	-1.291052	2.999797	-1.52995	C	-5.234462	-0.770843	-2.923179
C	-4.122639	-1.78754	-3.256189	H	-5.253613	-0.53974	-1.856384
C	4.041104	5.859272	-1.741417	H	-5.116746	0.167495	-3.474426
H	4.860941	5.975048	-2.45934	H	-6.212529	-1.186825	-3.190834

Table S4. Cartesian coordinates of **LSb(III)-monomer** in the S_0 state.

atom	x	y	z
Sb	-0.014435	-0.262081	-0.819708
O	-1.274719	-1.38169	0.335355
O	1.266398	-1.551922	0.125946
N	-1.456863	1.277816	-0.173724
N	1.377056	1.211192	0.004901
C	-0.00723	4.768399	0.157165
C	-0.033688	3.275907	0.048978
C	-1.273594	2.657846	-0.097418
C	-2.79511	1.029755	-0.180849
C	1.184175	2.594257	0.144498
C	-3.380836	-0.296067	-0.160751
C	3.348621	-0.344484	0.065372
C	2.611571	-1.552394	0.062651
C	-2.618336	-1.434245	0.202193
C	-4.770197	-0.415764	-0.379303
H	-5.309122	0.464258	-0.704695
C	-0.1633	5.382566	1.413669
C	3.313017	-2.792938	0.024998
C	0.165443	5.544706	-1.003305
C	-3.294916	-2.656779	0.477516
C	-2.555084	3.276828	-0.071562
H	-2.722495	4.341144	0.017347
C	-3.498276	2.271461	-0.116356
H	-4.570711	2.384763	-0.058987
C	2.711191	0.954667	0.185774
C	4.703346	-2.75472	-0.028435
H	5.237772	-3.694553	-0.065619
C	-4.670244	-2.700754	0.262688
H	-5.182969	-3.635653	0.445323
C	2.569075	-4.136084	0.010955
C	-2.540404	-3.896948	0.978083
C	4.758691	-0.380125	-0.011485
H	5.290169	0.560354	-0.050581
C	0.032163	7.5728	0.349406
C	-5.437292	-1.612112	-0.19184
C	2.438466	3.185485	0.443274
H	2.587893	4.238901	0.63331
C	5.460661	-1.569834	-0.058062
C	0.179668	6.937004	-0.886445
H	0.308308	7.538614	-1.78359
C	-0.140714	6.778373	1.486035
H	-0.262591	7.255566	2.45593
C	3.377634	2.176113	0.483999
H	4.424657	2.278677	0.725362
C	-1.564486	-4.36631	-0.118282
H	-0.830261	-3.595029	-0.337954
H	-1.029629	-5.265847	0.205973
H	-2.10973	-4.608073	-1.038533
C	6.989538	-1.64495	-0.144279
C	-6.940519	-1.788552	-0.435403
C	1.737159	-4.232084	-1.287082
H	2.40057	-4.225006	-2.159967
H	1.158772	-5.162766	-1.305657
H	1.042327	-3.397756	-1.378182
C	-0.354237	4.554456	2.661756
H	-1.271915	3.957879	2.607522
H	0.472847	3.849512	2.801675
H	-0.413932	5.192148	3.548343
C	-3.485304	-5.071091	1.29311
H	-4.017817	-5.425834	0.403195
H	-2.893436	-5.90944	1.676199
H	-4.224911	-4.81025	2.058763
C	0.327702	4.886714	-2.352469
H	0.424369	5.634552	-3.144722
H	1.217176	4.246479	-2.376619
H	-0.531133	4.247654	-2.58808
C	-1.78182	-3.555212	2.28024
H	-2.490959	-3.273477	3.067742
H	-1.219017	-4.429435	2.627675

H	-1.085105	-2.7306	2.130117
C	3.528131	-5.341299	0.022487
H	4.163678	-5.351032	0.915235
H	2.937894	-6.264171	0.026766
H	4.173265	-5.368611	-0.863041
C	7.533989	-2.413071	1.079852
H	8.627443	-2.484246	1.032561
H	7.262939	-1.901902	2.010239
H	7.134385	-3.431084	1.129344
C	-7.627584	-2.219625	0.878751
H	-7.222582	-3.163674	1.257198
H	-7.488219	-1.460353	1.656252
H	-8.704267	-2.356609	0.721051
C	7.395835	-2.386512	-1.436532
H	6.991992	-3.403777	-1.46292
H	7.024969	-1.856234	-2.320739
H	8.487782	-2.457334	-1.511377
C	0.084924	9.077516	0.456886
H	-0.291903	9.557033	-0.452616
H	-0.507724	9.439143	1.303608
H	1.114877	9.42755	0.606735
C	1.679685	-4.250877	1.266894
H	0.956354	-3.439973	1.319036
H	1.138986	-5.2043	1.261843
H	2.301298	-4.220549	2.169698
C	-7.160438	-2.876296	-1.509315
H	-8.231717	-3.024361	-1.691984
H	-6.687606	-2.588805	-2.454992
H	-6.736822	-3.838101	-1.202596
C	-7.604425	-0.490091	-0.921923
H	-7.507811	0.314479	-0.184149
H	-7.171194	-0.143805	-1.867005
H	-8.673648	-0.660697	-1.088712
C	7.638357	-0.251303	-0.164891
H	8.727798	-0.35085	-0.223213
H	7.311483	0.334785	-1.031221
H	7.404575	0.316684	0.742689

Table S5. Cartesian coordinates of **LSb(III)-dimer** in the S_0 state.

atom	x	y	z
Sb	2.292349	-0.111735	0.499808
O	1.072053	0.302589	2.101093
O	3.187799	1.52984	1.378993
N	1.778581	-2.159885	1.207899
N	4.30874	-0.933514	0.756019
C	4.482461	-4.745636	0.577926
C	3.85373	-3.393155	0.714472
C	2.483971	-3.33791	0.965139
C	0.516036	-2.498226	1.585457
C	4.698334	-2.278141	0.663953
C	-0.485896	-1.550205	2.038125
C	5.486513	1.286469	0.711041
C	4.375557	2.081846	1.08327
C	-0.14331	-0.21064	2.358676
C	-1.793432	-2.02386	2.291474
H	-2.030349	-3.038569	2.007107
C	4.930539	-5.421119	1.729233
C	4.542258	3.498403	1.169535
C	4.616206	-5.332916	-0.692528
C	-1.107397	0.605678	3.020242
C	1.605584	-4.438715	1.177934
H	1.886802	-5.478631	1.088958
C	0.389439	-3.921945	1.569819
H	-0.488844	-4.480876	1.853298
C	5.441472	-0.165443	0.704886
C	5.778895	4.034361	0.822172
H	5.899934	5.108114	0.870092
C	-2.3704	0.070119	3.255857
H	-3.099787	0.690182	3.757439
C	3.393563	4.42283	1.598036
C	-0.766504	2.028263	3.481497
C	6.704442	1.901745	0.345994
H	7.510909	1.268078	0.005557
C	5.663	-7.286191	0.331515
C	-2.758274	-1.232896	2.89363
C	6.113633	-2.321586	0.572942
H	6.696085	-3.230439	0.521189
C	6.875803	3.271916	0.383417
C	5.204684	-6.596409	-0.793817
H	5.305336	-7.051781	-1.776587
C	5.513455	-6.682981	1.583386
H	5.858706	-7.207092	2.471882
C	6.574775	-1.022347	0.612498
H	7.606211	-0.704499	0.606206
C	-0.429595	2.893533	2.250775
H	0.436069	2.50186	1.722366
H	-0.206912	3.922097	2.555201
H	-1.27683	2.922995	1.556447
C	8.175878	3.971248	-0.029028
C	-4.152029	-1.746056	3.277451
C	2.26784	4.346594	0.546806
H	2.629798	4.730972	-0.414524
H	1.407598	4.952145	0.852005
H	1.926214	3.323557	0.400583
C	4.783495	-4.801409	3.09824
H	3.730049	-4.627467	3.345197
H	5.285184	-3.828747	3.151049
H	5.211975	-5.449535	3.86805
C	-1.938777	2.70002	4.219248
H	-2.827981	2.792946	3.588264
H	-1.638765	3.710686	4.51671
H	-2.21638	2.156339	5.129436
C	4.113937	-4.62029	-1.923171
H	4.369009	-5.171925	-2.832551
H	4.540201	-3.613734	-2.001831
H	3.025463	-4.502313	-1.893888
C	0.418069	1.967839	4.471711
H	0.133991	1.388755	5.358445
H	0.689646	2.977614	4.79907

H	1.291967	1.500648	4.018777	H	9.517807	2.268387	0.300407
C	3.824646	5.898151	1.694501	Sb	-2.292086	0.111656	-0.50027
H	4.632155	6.043388	2.420973	O	-1.072568	-0.301321	-2.102469
H	2.96864	6.495739	2.026739	O	-3.187042	-1.53021	-1.379404
H	4.150238	6.30113	0.728654	N	-1.77888	2.160419	-1.207321
C	8.737099	4.760523	1.173658	N	-4.308583	0.932916	-0.756382
H	9.664552	5.275862	0.895786	C	-4.48369	4.744982	-0.577012
H	8.95511	4.088093	2.010708	C	-3.854382	3.392813	-0.713985
H	8.027761	5.515623	1.527655	C	-2.484565	3.338174	-0.964331
C	-4.184372	-1.949954	4.809053	C	-0.516469	2.499114	-1.584821
H	-3.975215	-1.01453	5.339532	C	-4.698589	2.277434	-0.664079
H	-3.434419	-2.686111	5.119178	C	0.485534	1.551346	-2.037906
H	-5.170915	-2.308416	5.127788	C	-5.485835	-1.287425	-0.711688
C	7.888966	4.945749	-1.192061	C	-4.37463	-2.082546	-1.083686
H	7.146094	5.700452	-0.91472	C	0.143002	0.211951	-2.359248
H	7.505233	4.405017	-2.064107	C	1.793026	2.025219	-2.290962
H	8.805538	5.469689	-1.489234	H	2.029853	3.039669	-2.005618
C	6.326561	-8.635252	0.196602	C	-4.932441	5.42047	-1.728111
H	5.946763	-9.182775	-0.672293	C	-4.54089	-3.499147	-1.169803
H	6.163163	-9.252156	1.086451	C	-4.617402	5.331926	0.693548
H	7.412043	-8.531186	0.067328	C	1.107301	-0.604095	-3.020804
C	2.885186	4.002628	2.991039	C	-1.606425	4.439272	-1.17678
H	2.547532	2.969371	2.990254	H	-1.887908	5.4791	-1.087584
H	2.051867	4.644575	3.299654	C	-0.390156	3.922881	-1.568784
H	3.685728	4.107458	3.733031	H	0.488018	4.482061	-1.852132
C	-5.236565	-0.720854	2.885376	C	-5.441142	0.164503	-0.705583
H	-6.230665	-1.117797	3.122223	C	-5.777416	-4.035426	-0.822535
H	-5.208673	-0.506942	1.815449	H	-5.898139	-5.109223	-0.870336
H	-5.124601	0.225053	3.424909	C	2.370166	-0.068186	-3.256465
C	-4.4815	-3.083742	2.596666	H	3.099645	-0.687936	-3.758289
H	-3.797832	-3.879719	2.912907	C	-3.391843	-4.423215	-1.598132
H	-4.441923	-3.00669	1.507781	C	0.766914	-2.026936	-3.481702
H	-5.494175	-3.39745	2.87041	C	-6.703653	-1.902999	-0.346757
C	9.247671	2.972388	-0.494731	H	-7.510365	-1.269526	-0.006544
H	10.1564	3.511662	-0.783843	C	-5.665611	7.284812	-0.329802
H	8.911581	2.396192	-1.364316	C	2.757858	1.234741	-2.893798

C	-6.11391	2.32043	-0.573357	H	-4.629885	-6.044494	-2.420488
H	-6.696637	3.229097	-0.521463	H	-2.966124	-6.496052	-2.026397
C	-6.874617	-3.27323	-0.38406	H	-4.14761	-6.301608	-0.728179
C	-5.206642	6.595081	0.795238	C	-8.735619	-4.762052	-1.17461
H	-5.307368	7.050171	1.778125	H	-9.662965	-5.277637	-0.896838
C	-5.516001	6.681942	-1.581877	H	-8.95377	-4.089511	-2.011535
H	-5.86176	7.206048	-2.470185	H	-8.026125	-5.516939	-1.528748
C	-6.574679	1.021067	-0.613316	C	4.183616	1.952715	-4.809133
H	-7.606026	0.702926	-0.607282	H	3.974591	1.017426	-5.339903
C	0.429844	-2.891757	-2.250705	H	3.433499	2.688836	-5.118948
H	-0.436572	-2.500471	-1.723248	H	5.170067	2.311466	-5.127828
H	0.208267	-3.920694	-2.554668	C	-7.887501	-4.947557	1.191082
H	1.276518	-2.920054	-1.555665	H	-7.144537	-5.702108	0.913578
C	-8.174571	-3.972886	0.028226	H	-7.503815	-4.406936	2.063216
C	4.151455	1.748313	-3.277594	H	-8.803996	-5.471675	1.488178
C	-2.266144	-4.346245	-0.546925	C	-6.329952	8.633466	-0.194657
H	-2.628074	-4.730163	0.414575	H	-5.956301	9.177719	0.678915
H	-1.405755	-4.951755	-0.851767	H	-6.16012	9.253631	-1.081058
H	-1.924748	-3.323075	-0.401096	H	-7.416362	8.529101	-0.073687
C	-4.785444	4.801041	-3.097249	C	-2.883738	-4.003171	-2.991289
H	-3.732048	4.626568	-3.34402	H	-2.546856	-2.969651	-2.99095
H	-5.28767	3.82867	-3.150418	H	-2.049928	-4.644607	-3.29963
H	-5.213414	5.449598	-3.866979	H	-3.684192	-4.108926	-3.733247
C	1.939622	-2.698632	-4.218788	C	5.236246	0.723221	-2.885946
H	2.82886	-2.79049	-3.587676	H	6.230247	1.120484	-3.122662
H	1.640233	-3.709686	-4.515545	H	5.208429	0.508911	-1.816094
H	2.217029	-2.155472	-5.129356	H	5.124461	-0.222501	-3.425836
C	-4.113994	4.619642	1.923936	C	4.480598	3.08586	-2.596395
H	-4.373053	5.168765	2.833718	H	3.796734	3.881739	-2.912451
H	-4.535765	3.61106	2.000351	H	4.440854	3.008452	-1.507549
H	-3.024899	4.506797	1.896344	H	5.493219	3.399935	-2.869917
C	-0.417467	-1.967376	-4.472194	C	-9.246566	-2.974315	0.494083
H	-0.133466	-1.388537	-5.359114	H	-10.15523	-3.513807	0.782993
H	-0.688572	-2.977397	-4.799194	H	-8.910642	-2.398271	1.363833
H	-1.291641	-1.500361	-4.019596	H	-9.51675	-2.270169	-0.300911
C	-3.822327	-5.898734	-1.694176				

Table S6. Cartesian coordinates of **LSb(V)Cl_2** in the S_0 state.

atom	x	y	z
C	5.508626	-1.532063	-0.044352
C	4.767546	-2.722533	-0.041447
C	3.377223	-2.772424	-0.161763
C	2.68605	-1.545635	-0.303517
C	3.398417	-0.319312	-0.323986
C	4.800362	-0.348996	-0.185226
H	5.29863	-3.655698	0.066062
H	5.334205	0.592396	-0.164484
C	2.767308	0.984974	-0.434634
C	3.423342	2.238688	-0.595516
C	2.472766	3.234016	-0.495366
H	4.480238	2.377019	-0.763535
C	1.214262	2.615387	-0.277685
H	2.624183	4.302172	-0.554136
C	0.001576	3.251713	0.000042
C	-1.21167	2.616455	0.27774
N	-1.428014	1.233151	0.291931
C	-2.469612	3.236234	0.495543
C	-2.766192	0.987446	0.434581
C	-3.42108	2.241755	0.595599
H	-2.620118	4.304528	0.554429
C	-3.398475	-0.316256	0.32384
H	-4.477845	2.381037	0.763663
C	-2.687218	-1.543227	0.303434
C	-4.800434	-0.344649	0.184969
C	-3.379505	-2.769387	0.161656
C	-5.50977	-1.527073	0.044067
H	-5.333401	0.597238	0.164155
C	-4.769776	-2.718216	0.041254
H	-5.301707	-3.650904	-0.066241
C	0.002289	4.748366	0.0001
C	0.264253	5.441354	1.196171
C	-0.264589	5.441752	-1.194714
C	0.255584	6.838727	1.173838
C	-0.263175	6.839074	-1.170352
C	-0.002338	7.555038	0.001555
H	0.454397	7.3796	2.096314
H	-0.472627	7.380234	-2.090307
O	1.343468	-1.59666	-0.499921
O	-1.344689	-1.595435	0.499938
C	2.636184	-4.11915	-0.172833
C	-2.639772	-4.116829	0.172811
C	7.035469	-1.500156	0.112103
C	-7.036571	-1.493771	-0.112502
C	-0.553056	4.694272	-2.474573
H	0.281468	4.041065	-2.75331
H	-1.433537	4.049841	-2.371655
H	-0.733261	5.388199	-3.300328
C	0.546217	4.693519	2.47727
H	-0.291983	4.044581	2.755038
H	1.423727	4.044758	2.376454
H	0.728299	5.387233	3.302791
C	0.025883	9.064164	-0.004553
H	1.032251	9.439252	-0.232959
H	-0.652785	9.473931	-0.759788
H	-0.260314	9.47355	0.969772
C	-7.662638	-0.80828	1.121399
H	-7.302979	0.219149	1.240009
H	-8.754368	-0.771372	1.025583
H	-7.416891	-1.356402	2.037591
C	-7.640565	-2.902495	-0.237614
H	-7.259634	-3.431236	-1.118301
H	-7.432074	-3.514	0.647333
H	-8.72852	-2.827754	-0.340771
C	-7.401584	-0.696665	-1.383722
H	-7.0346	0.333786	-1.334528
H	-6.966166	-1.163876	-2.273737

H	-8.489981	-0.659266	-1.512481	C	3.592249	-5.307867	0.041036
C	-1.963283	-4.315501	1.548501	H	4.341172	-5.386839	-0.755075
H	-1.418723	-5.266842	1.563782	H	4.1125	-5.250384	1.003963
H	-1.261085	-3.513786	1.775681	H	3.009744	-6.23525	0.035612
H	-2.720032	-4.345789	2.341213	C	7.401318	-0.703277	1.383225
C	-1.601324	-4.160884	-0.968564	H	8.48976	-0.666876	1.511899
H	-0.85646	-3.374314	-0.874901	H	7.035285	0.32751	1.333969
H	-1.081139	-5.12539	-0.960163	H	6.965535	-1.170004	2.273314
H	-2.095386	-4.049544	-1.940434	C	7.662077	-0.815354	-1.121905
C	-3.59702	-5.304572	-0.041122	H	7.303354	0.212394	-1.240581
H	-4.346085	-5.382769	0.754931	H	8.75385	-0.779445	-1.026176
H	-4.11714	-5.246567	-1.004089	H	7.415756	-1.363331	-2.038029
H	-3.015457	-6.232546	-0.035643	C	7.638171	-2.909426	0.237297
C	1.597771	-4.162142	0.968602	H	7.256795	-3.437743	1.118046
H	0.853728	-3.374785	0.875003	H	7.429072	-3.52081	-0.647588
H	1.076574	-5.126101	0.96021	H	8.7262	-2.83568	0.340396
H	2.092011	-4.051342	1.940443	N	1.429342	1.231883	-0.291985
C	1.959371	-4.317137	-1.548463	Sb	-0.000004	-0.249355	-0.000012
H	1.413871	-5.26794	-1.563707	Cl	-0.643301	-0.253599	-2.330336
H	1.257941	-3.514725	-1.775561	Cl	0.643328	-0.254129	2.330315
H	2.716015	-4.348161	-2.341247				

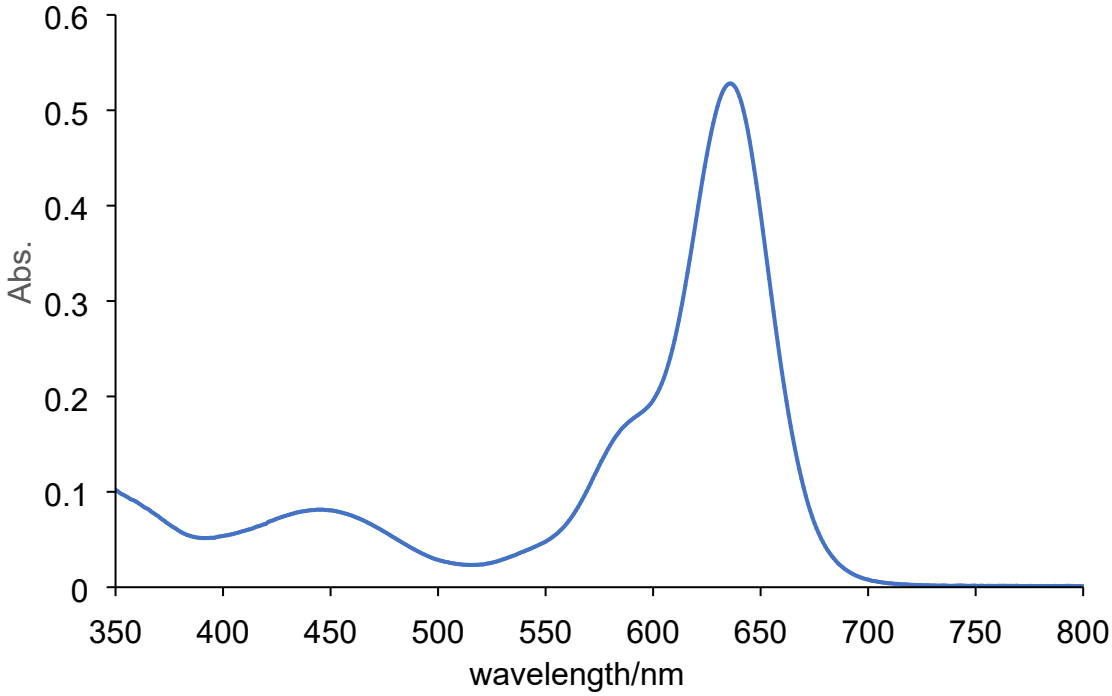


Figure S5. UV/vis spectra of **$LSbCl_2$** in acetone (1.0×10^{-5} M).

Stability tests of LSb(III) and LBi(III)

1. In the solid state

Powdered samples of **LSb(III)** or **LBi(III)** (1.0 mg) were kept under air and dark at 293 K for 1 d. The samples were dissolved in acetone-$\boldsymbol{d}_6$, and ^{1}H NMR spectra were measured to show no sign of decomposition.

2. In air- and moisture-saturated solvents

LSb(III) or **LBi(III)** (1.0 mg) were dissolved in acetone-$\boldsymbol{d}_6$ or $CDCl_3$ (0.5 mL), and the solutions were kept under dark at 293 K. ^{1}H NMR spectra of the acetone-$\boldsymbol{d}_6$ solutions showed no sign of decomposition after 1 d (Fig. S6 and S7). In $CDCl_3$, 7% of **LSb(III)** decomposed to $\mathbf{LH_3}$ after 1d (Fig. S8). In contrast, 13% of LBi(III) decomposed to LH3 just after the dissolution in CDCl3, and 23% of LBi(III) decomposed after 1 d (Fig. S9).

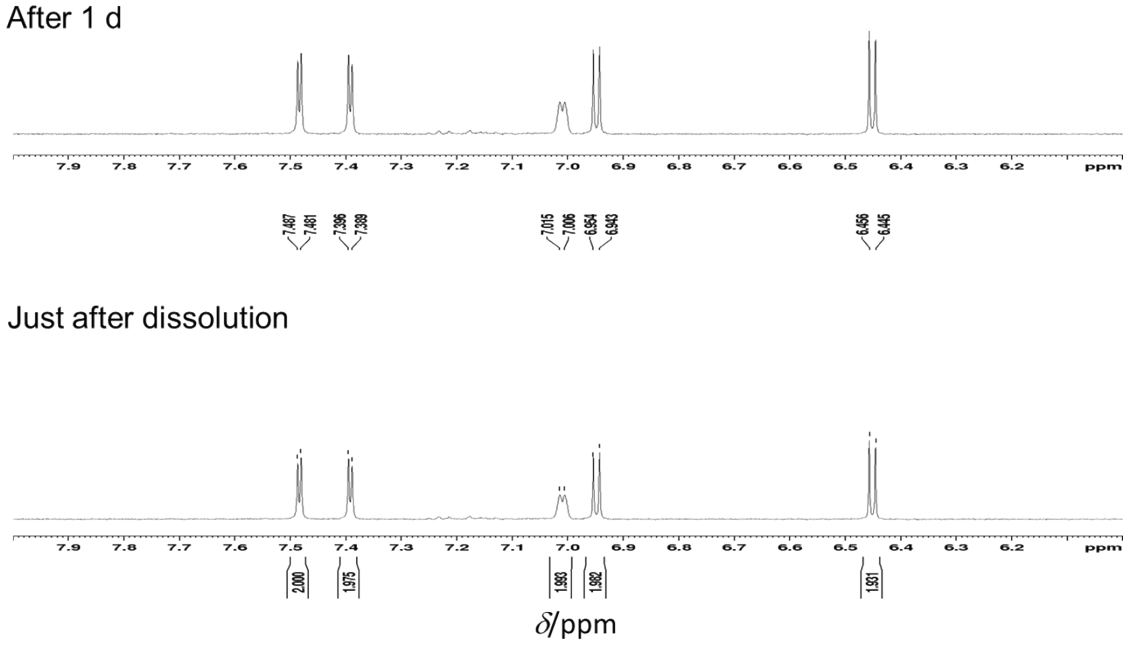


Figure S6. Aromatic region of the ^{1}H NMR spectra of **LSb(III)** in acetone-$\boldsymbol{d}_6$.

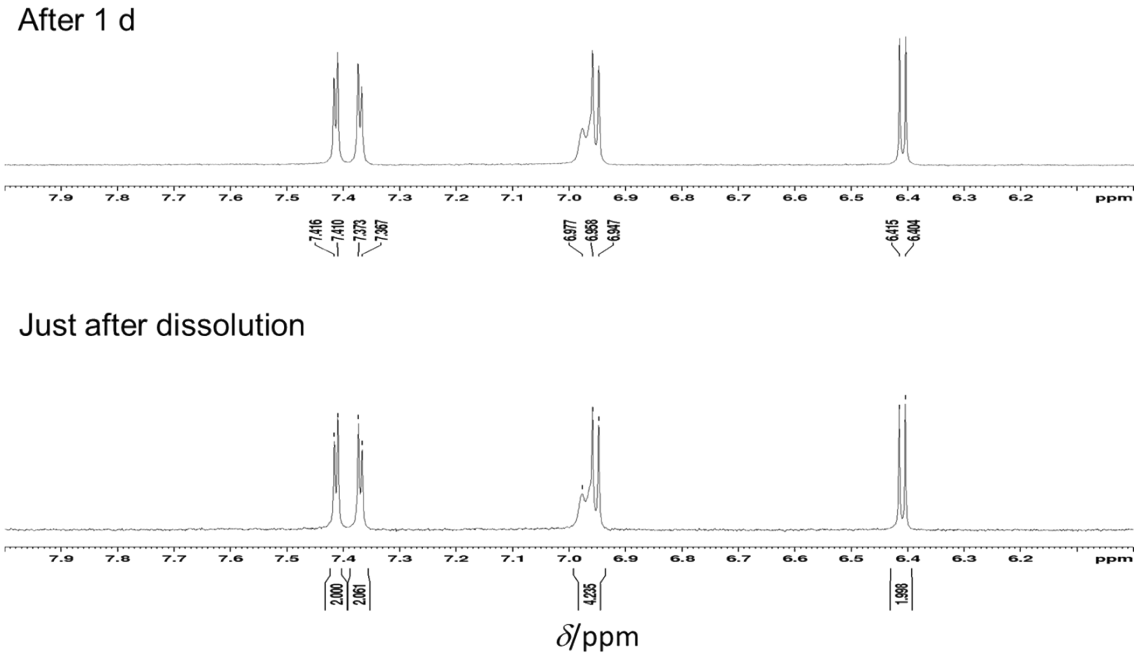


Figure S7. Aromatic region of the ^{1}H NMR spectra of **LBi(III)** in acetone-d_6.

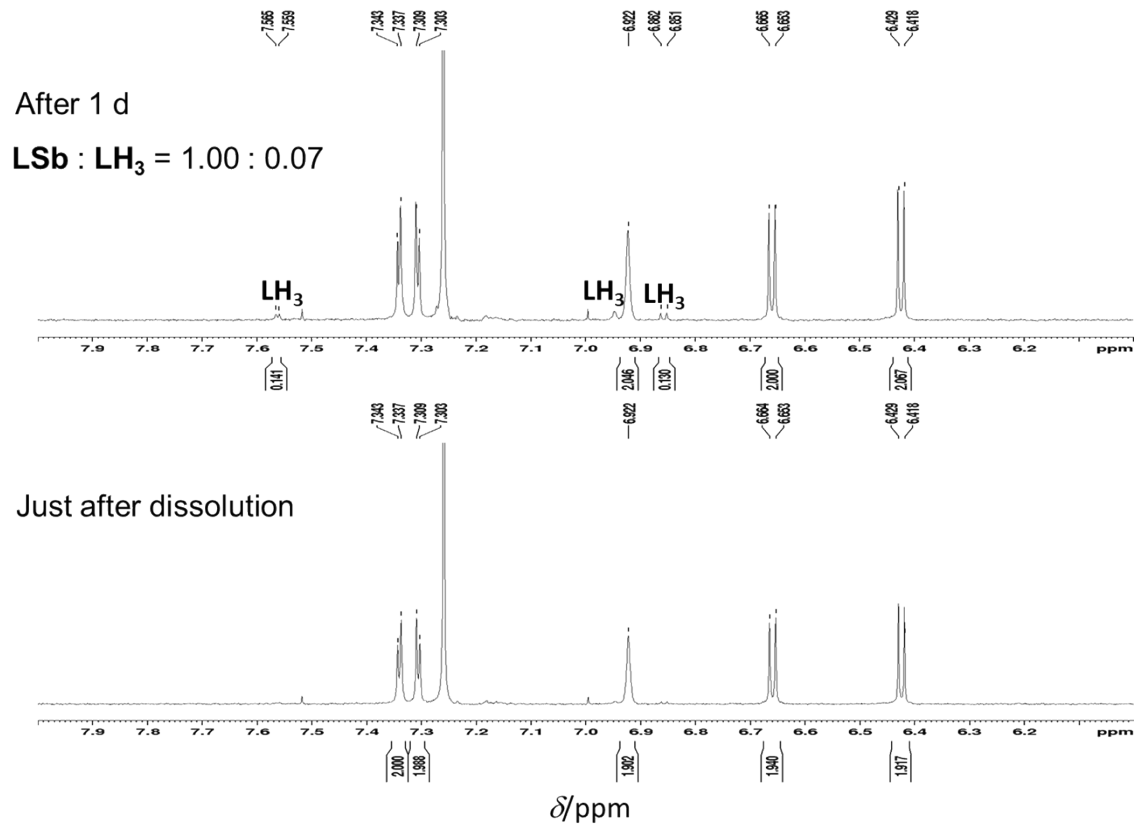


Figure S8. Aromatic region of the ^{1}H NMR spectra of **LSb(III)** in $CDCl_3$.

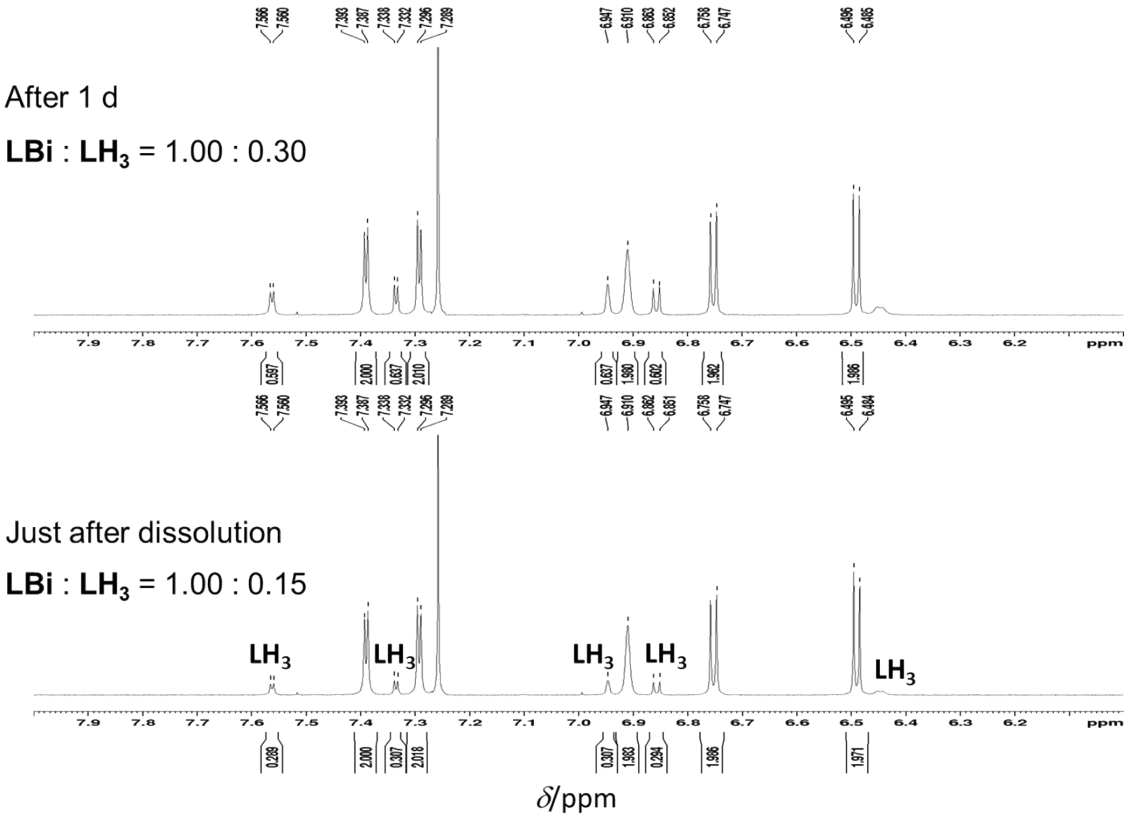


Figure S9. Aromatic region of the ^{1}H NMR spectra of **LBi(III)** in $CDCl_3$.

Optical spectra of **LSb(III)** and **LBi(III)**

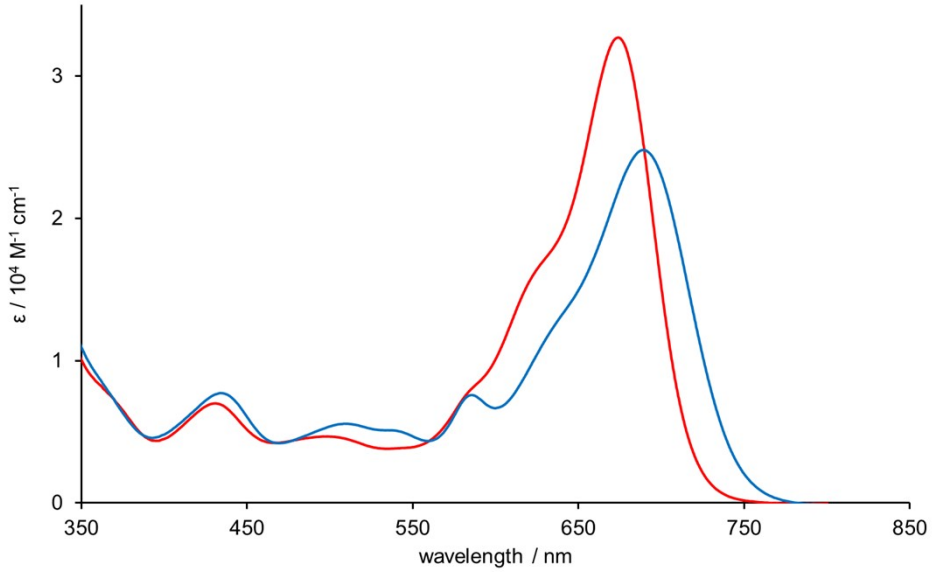


Figure S10. UV/vis spectra of **LSb(III)** (red line) and **LBi(III)** (blue line) in acetone (1.0×10^{-5} M, 293 K).

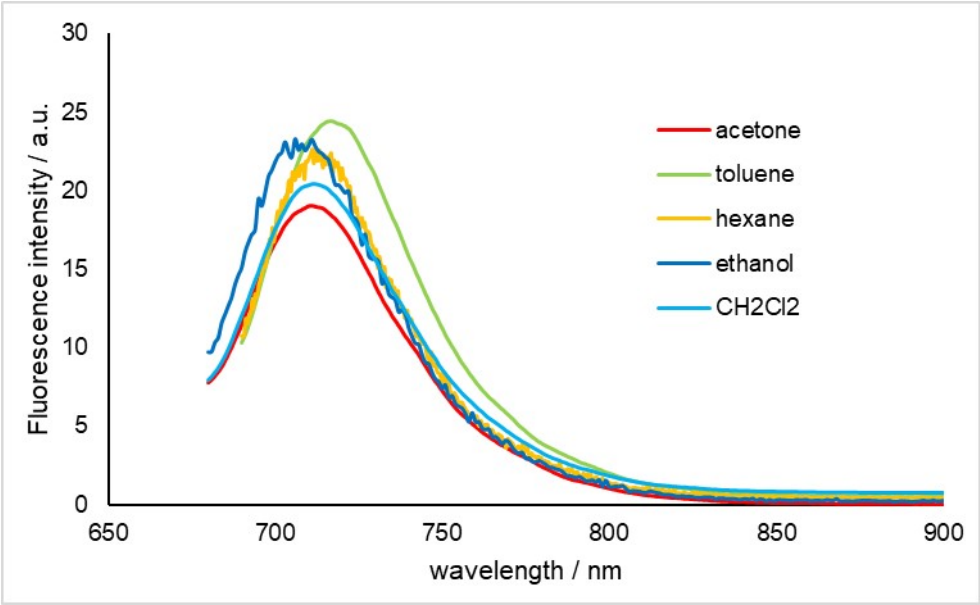


Figure S11. Fluorescence spectra of **LSb(III)** (1.0×10^{-5} M, 293 K, excitation: 675 nm).

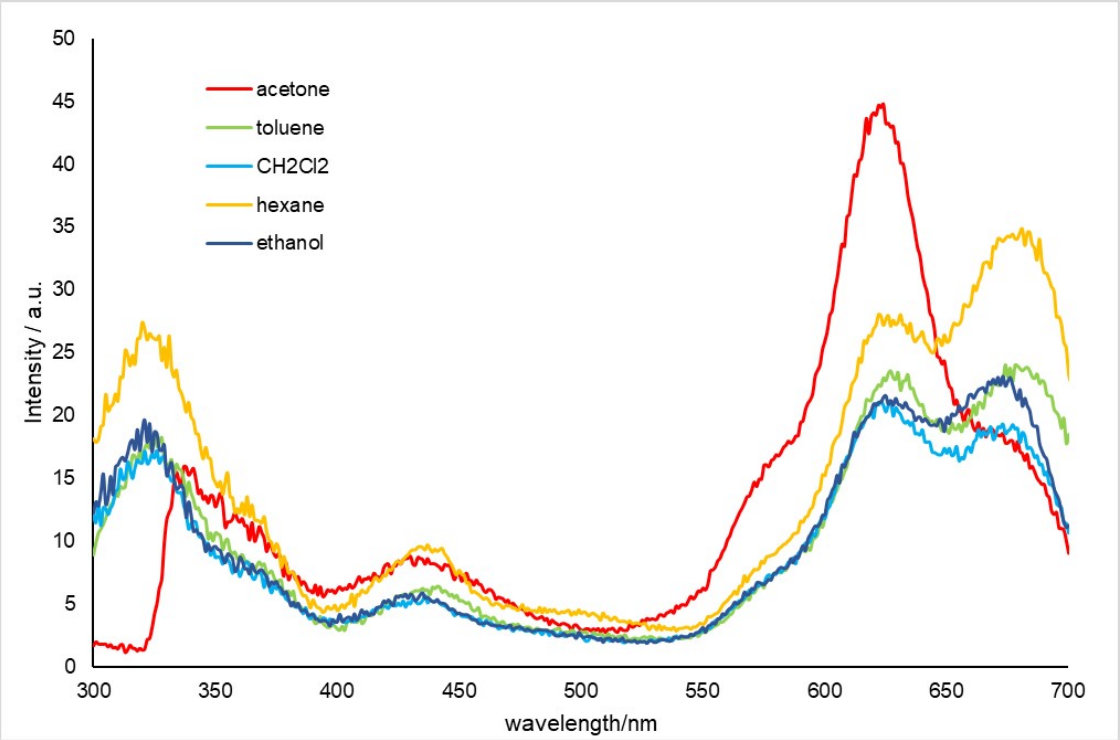


Figure S12. Excitation spectra of **LSb(III)** (1.0×10^{-5} M, 293 K, wavelength: 700 nm).

Table S7. Visible absorption wavelengths (nm) and molar absorption coefficients (M^{-1} cm^{-1}) of **LSb(III)** and **LBi(III)** in acetone.

	Absorption wavelength and molar absorption coefficients
LSb(III)	678 (3.27×10^4), 623 (1.61×10^4), 584 (0.75×10^4), 492 (0.50×10^4), 425 (0.72×10^4)
LBi(III)	689 (2.48×10^4), 639 (1.30×10^4), 578 (0.76×10^4), 512 (0.55×10^4), 436 (0.77×10^4)

References

S1 T. Agou, S. Kuroiwa, H. Fukumoto and T. Nabeshima, *Chem. Commun.*, 2024, **60**, 4557.

S2 O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Cryst*., 2009, **42**, 339-341.

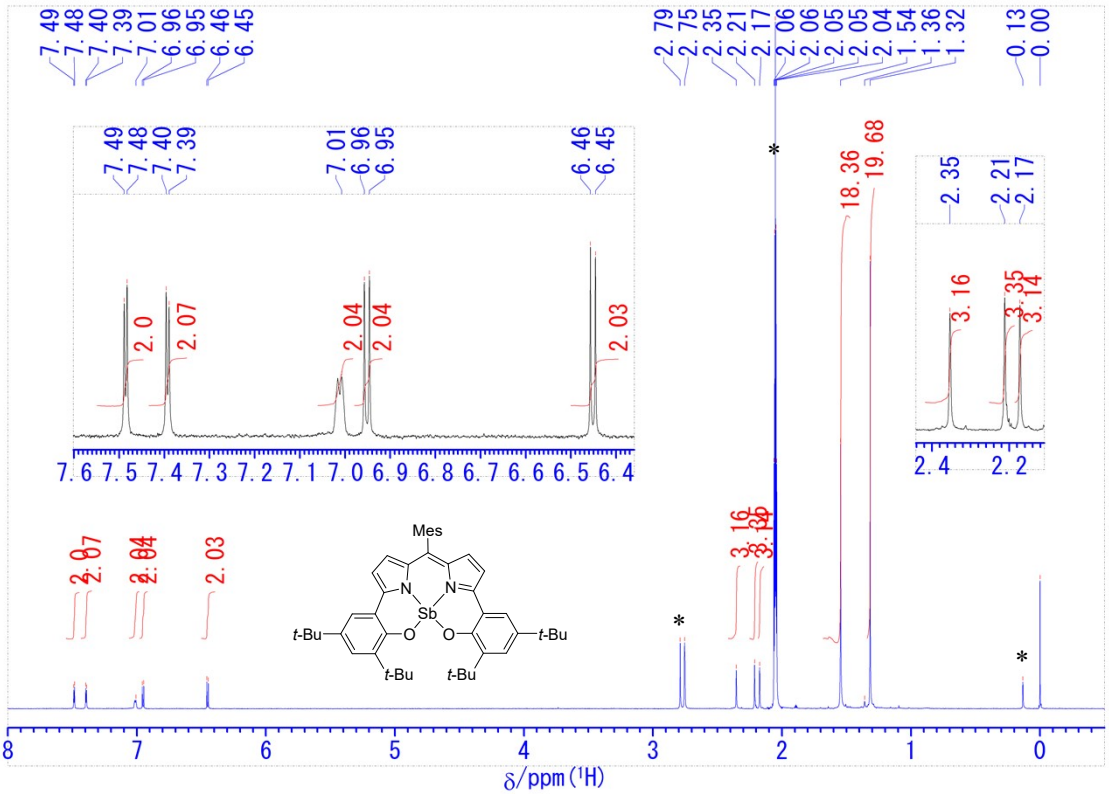
S3 (a) G. M. Sheldrick, *Acta Cryst. A*, 2008, **64**, 112-122; (b) G. M. Sheldrick, *Acta Cryst. C*, 2015, **71**, 3-8

S4 Gaussian 16, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2019.

^{1}H and ^{13}C NMR spectra and HRMS data of newly synthesized compounds

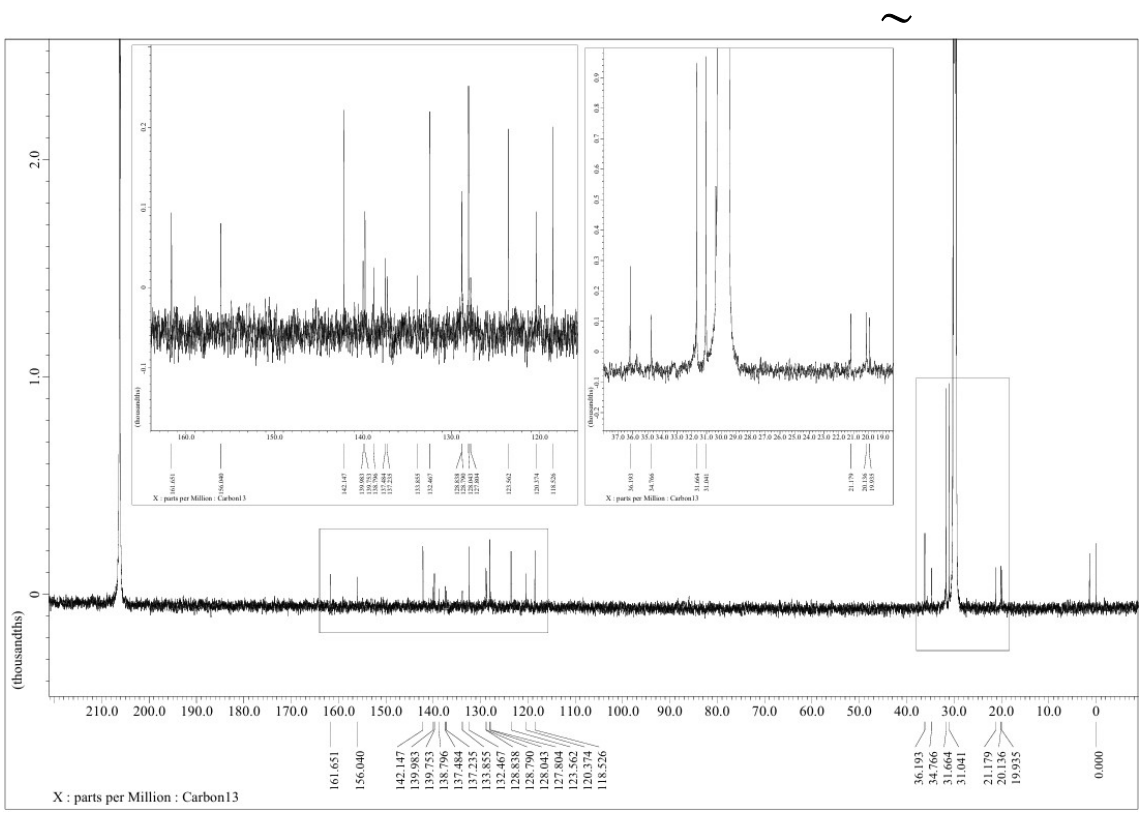
LSb

^{1}H NMR (400 MHz, acetone-d_6)

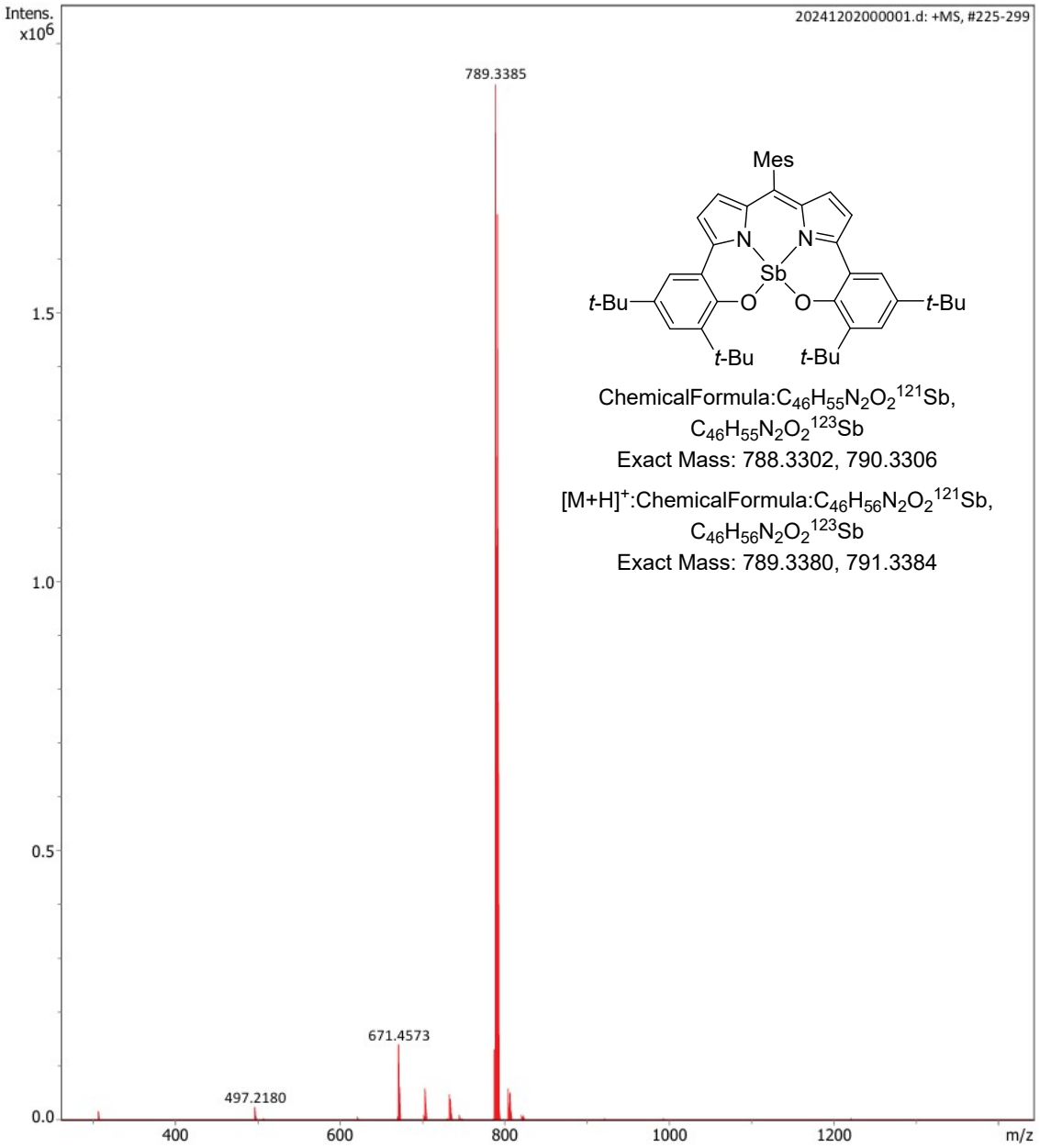


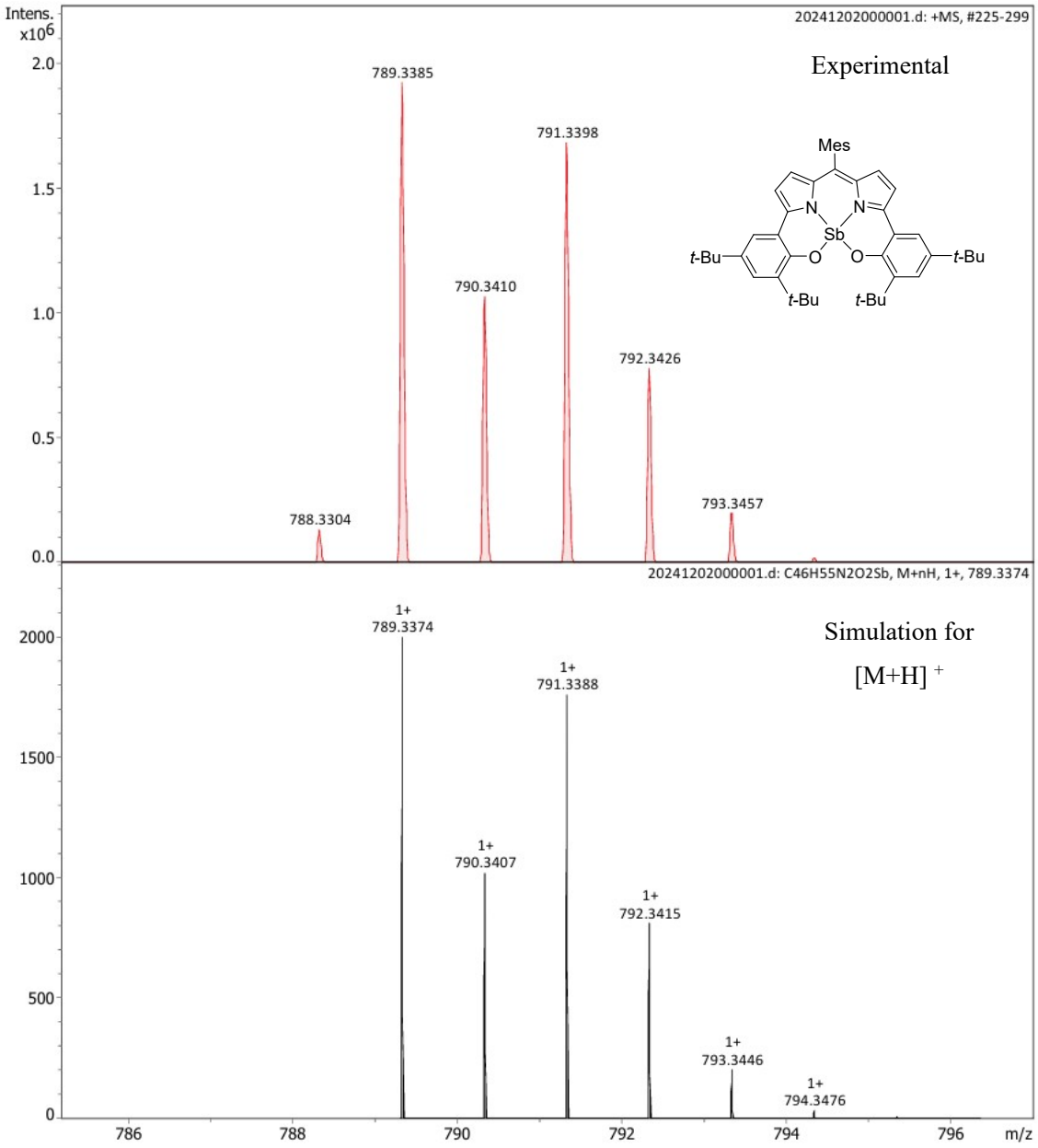
*Signals corresponding to residual solvent, silicone grease, and water.

^{13}C NMR (150 MHz, acetone-$\boldsymbol{d}_6$)



HRMS (APCI-pos, solvent: acetone)




Intens.
x10^6
20241202000001.d: +MS, #225-299
Experimental
789.3385
791.3398
790.3410
792.3426
788.3304
793.3457
Mes
N
N
Sb
O
O
t-Bu
t-Bu
t-Bu
t-Bu
20241202000001.d: C46H55N2O2Sb, M+nH, 1+, 789.3374
Simulation for
[M+H] +
1+
789.3374
1+
791.3388
1+
790.3407
1+
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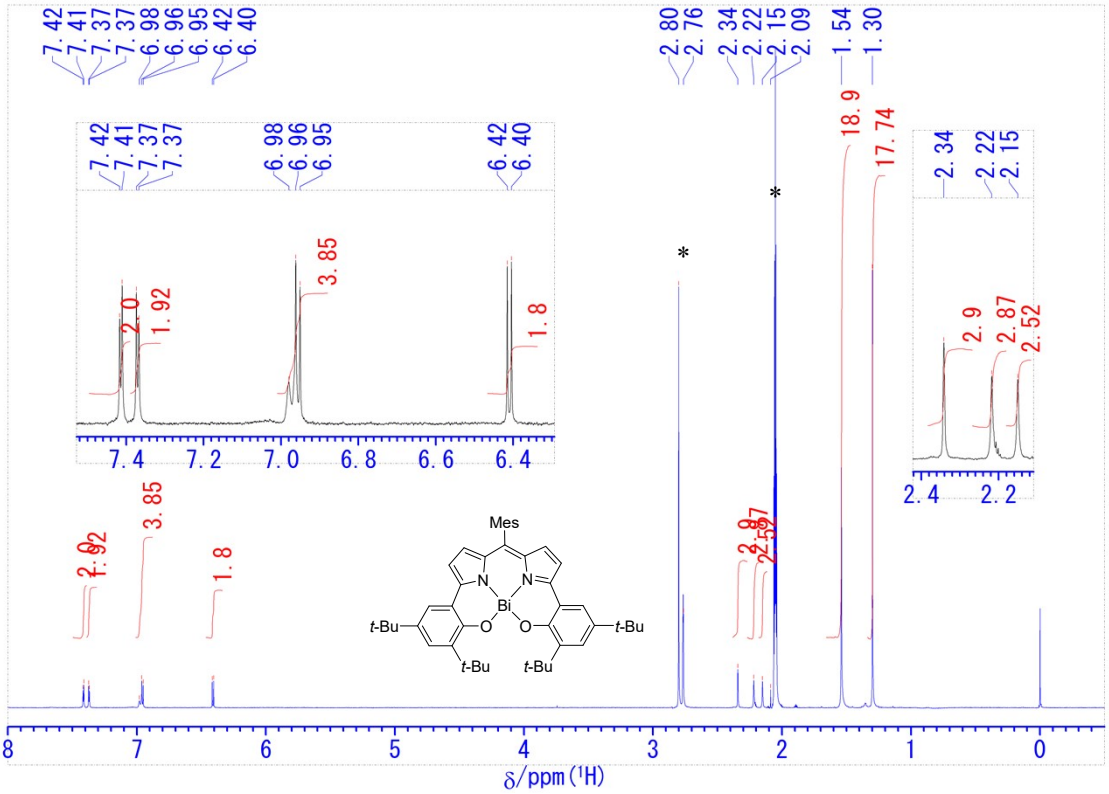
1+
793.3446
1+
794.3476
m/z

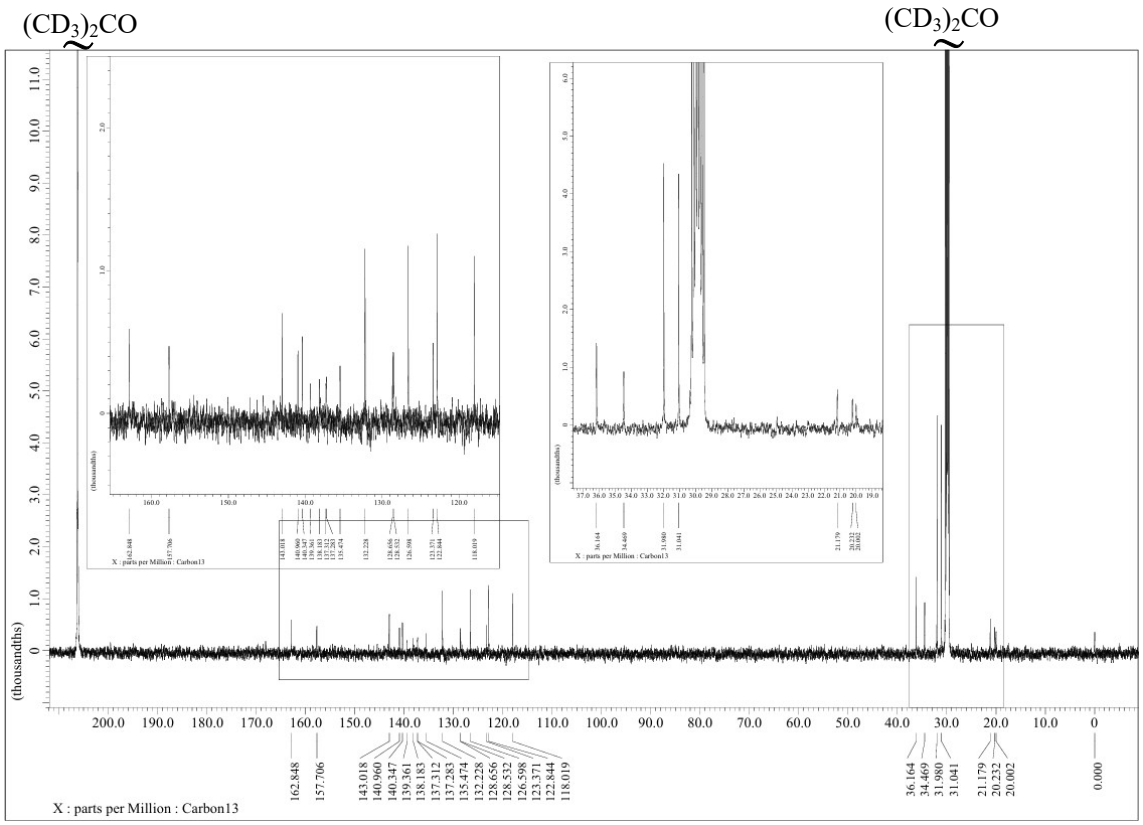
LBi

^{1}H NMR (400 MHz, acetone-d_6)

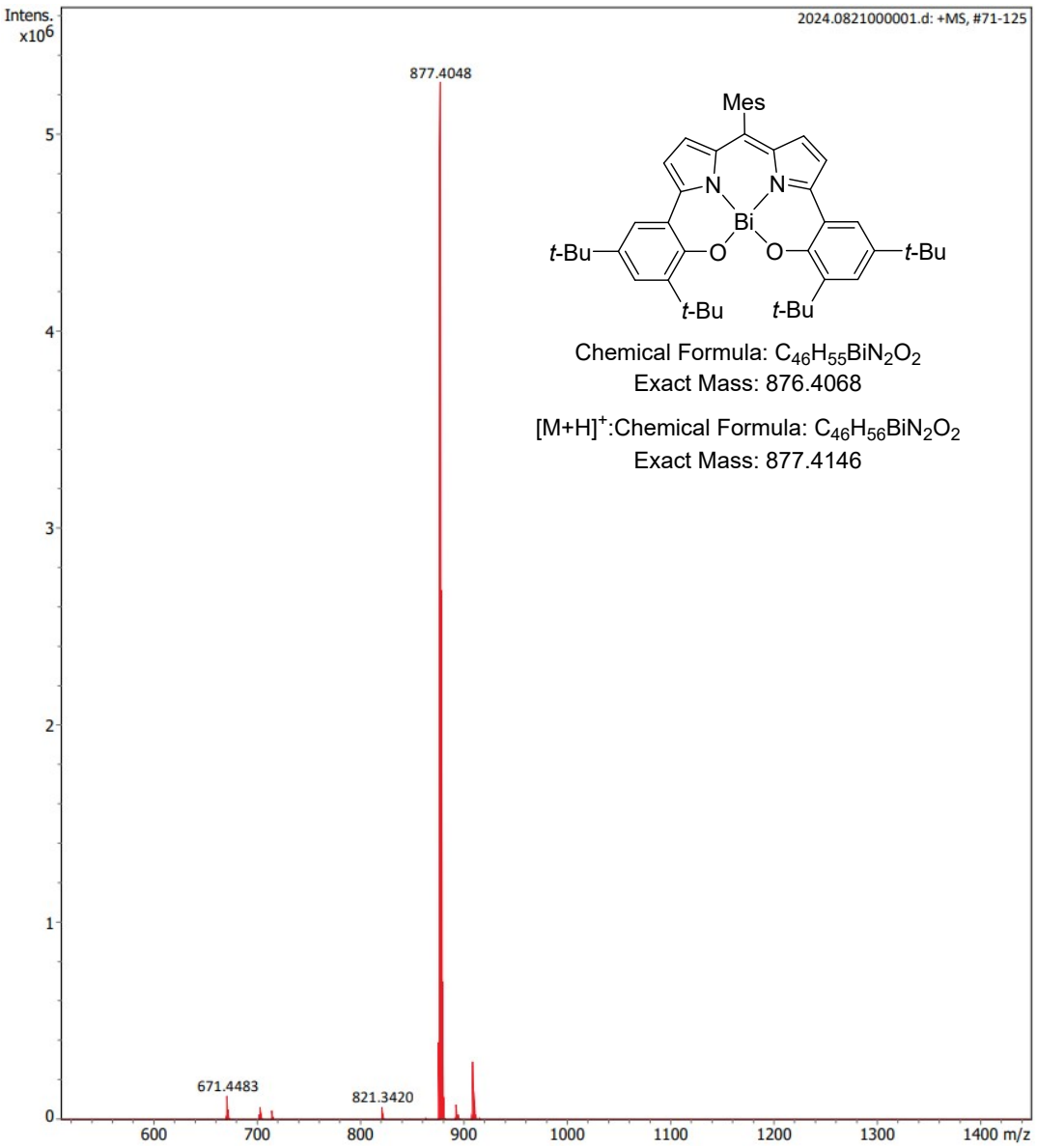


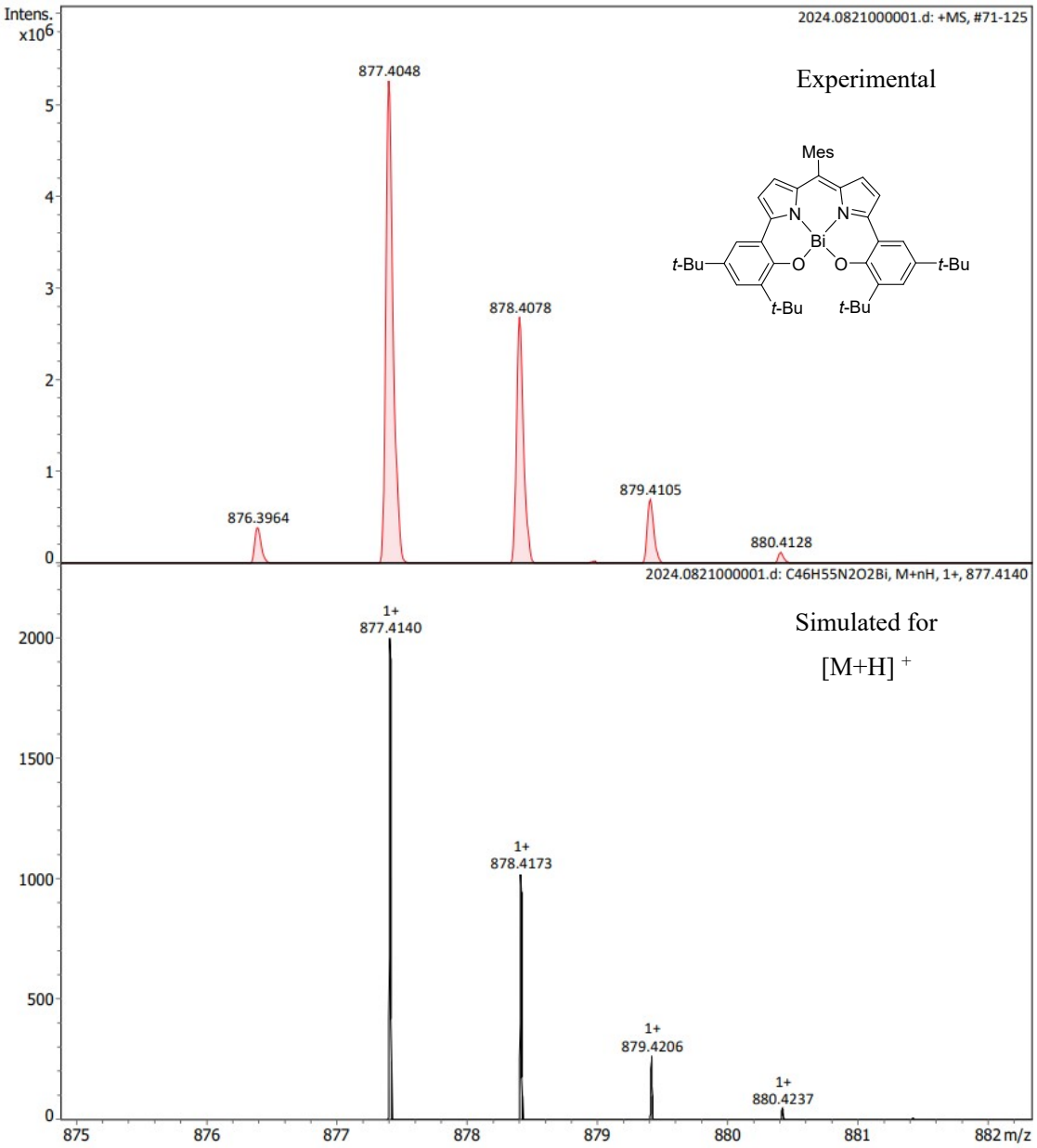
*Signals corresponding to residual solvent and water.

^{13}C NMR (150 MHz, acetone-$\boldsymbol{d}_6$)



HRMS (APCI-pos, solvent: acetone)





Simulated for