Electronic Supplementary Information

Synthesis of an amidinate-supported arsasilene and its attempted oxidation

Jicheng Wang,[a,‡] Yufen Yang,[a,‡] Zhicheng Xiao,[a] Manbo Zhang[a] and Bin Li*[a]

[a] Key Laboratory of Chemical Biology and Traditional Chinese Medicine Research, Key Laboratory of Light Energy Conversion Materials of Hunan Province, Key Laboratory of Phytochemical R&D of Hunan Province, College of Chemistry and Chemical Engineering, Hunan Normal University Changsha 410081, P. R. China.

[‡] These authors contributed equally to this work.

* E-mail: binli@hunnu.edu.cn

Content

I. Experimental Section

General procedure: All manipulations were carried out under an atmosphere of dry argon using standard Schlenk-line system and glovebox techniques. Deuterated benzene, toluene, and *n*-hexane were dried by refluxing with sodium under argon and stored with 4Å molecular sieve. Fluorobenzene was dried with CaH_2. NMR (^{1}H, $^{13}C\{^{1}H\}$, ^{29}Si, ^{11}B, $^{19}F$and 2D) spectra were collected on a Bruker Avance II 500 and 700 MHz spectrometers. IR spectra were recorded on Shimadzu IRTracer-100/AIM-9000 instrument. High-resolution mass spectrometry (HRMS) was conducted using a Shimadzu LCMS9030 system. Cyclic voltammograms was recorded on CHI 660E A14099 instrument. Ultraviolet visible (UV-vis) spectra were collected with a Shimadzu UV-2600i UV-vis spectrophotometer. Commercial reagents were purchased and used as received. (L)SiCl (L = $PhC(N^{t}Bu)_2$)[S1] was prepared according to literature methods.

Synthesis of 1: Na (1.50 g, 65.0 mmol) and grey arsenic (1.52 g, 20.0 mmol) were suspended in DME (100 mL), and naphthalene (100 mg, 0.8 mmol) was added. The solution was refluxed for 72 h under stirring. After cooling down to room temperature, a solution of iPr_3SiCl (12.2 g, 65.3 mmol) in DME (50 mL) was added dropwise to the Na_3As solution. The resulting suspension was further refluxed for 48 h. Then the suspension was filtered to remove insoluble impurities, and the solvent was removed in vacuo. Compound **1** was precipitated by adding toluene (200 mL), and isolated as white solid by filtration. (1.48 g, 19%). **^{1}H NMR (500 MHz, THF-d_8)**: δ 0.97-1.24 (m, 42H, C*H*Me_2 and CH*Me*$_2$); **$^{13}C\{^{1}H\}$ NMR (125 MHz, THF-d_8)**: δ 17.3 (s, *C*HMe_2), 21.3 (s, CH*Me*$_2$); **^{29}Si NMR (100 MHz, THF-d_8)**: δ 24.0 (iPr_3*Si*). HRMS (m/z): [**1**+H]$^+$ calcd for $C_{18}H_{43}AsNaSi_2^+$: 413.2011; found, 413.1979. Note: *The reaction was carried out in the absence of light to prevent the decomposition.*

Synthesis of 2: To the mixture of LSiCl (110 mg, 0.37 mmol) and $NaAs(Si^{i}Pr_3)_2$ (155 mg, 0.38 mmol) was added toluene (30 mL) at room temperature. The solution was stirred for 24 h. After filtration, the filtrate was dried under vacuum to afford **2** as yellow solid (230 mg, 96%). Single crystals suitable for X-ray diffraction analysis were grown from *n*-hexane solution at -30 °C. **^{1}H NMR (500 MHz, C_6D_6)**: δ 1.26 (s, 18H, *tBu*), 1.47 (m, 39H, C*H*Me_2 and CH*Me*$_2$), 1.82 (sept, $^{3}J_{HH}$ = 5 Hz, 3H, C*H*Me_2), 6.91-7.45 (m, 5H, *Ph*); **$^{13}C\{^{1}H\}$ NMR (125 MHz, C_6D_6)**: δ 14.5 (s, *C*HMe_2), 16.1 (s, *C*HMe_2), 20.8 (s, CH*Me*$_2$), 20.9 (s, CH*Me*$_2$), 32.0 (C*Me*$_3$), 55.3 (*C*Me_3), 127.8, 128.4, 128.8, 129.6, 130.4, 132.4 (*Ph*), 171.8 (N*C*N); **^{29}Si NMR (100 MHz, C_6D_6)**: δ -2.5 (iPr_3*Si*-Si), 25.4 (iPr_3*Si*-As), 36.5 (*Si*=As). HRMS (m/z): [**2**+H]$^+$ calcd for $C_{33}H_{66}N_2PSi_3^+$: 649.3744; found, 649.3751. **ATR-IR**: *v* 2929, 2856, 2158, 2029, 1973, 1448, 1402, 1356, 1263, 1197, 1082, 987, 879, 789, 754, 707, 642, 626, 574.

Synthesis of 3: To the solid mixture of **2** (150 mg, 0.20 mmol) and $[Ph_3C][B(C_6F_5)_4]$ (218 mg, 0.20 mmol) was added the pre-cooled fluorobenzene (12 mL). The solution was stirred for 1 h. The solution changed from yellow to reddish yellow. After removing the solvent under vacuum, the residue was washed with *n*-hexane (10 mL), to yield a crude product. Recrystallization by layering *n*-hexane on the top of

Fluorobenzene solution at room temperature gave single crystals of **3** (81 mg, 18%) with unidentified impurities. Unfortunately, attempts for complete purification was failed. **^{1}H NMR (500 MHz, C_6D_5Br)**: δ 0.21 (s, 1H, As*H*), 1.20 (s, 18H, *tBu*), 1.22-1.36 (m, 39H, C*H*Me$_2$ and CH*Me*$_2$), 1.61 (sept, $^{3}J_{HH}$ = 5 Hz, 3H, C*H*Me$_2$), 7.12-7.53 (m, 5H, *Ph*); **^{13}C{^{1}H} NMR (125 MHz, C_6D_5Br)**: δ 14.0 (s, *C*HMe$_2$), 14.9 (s, *C*HMe$_2$), 19.5 (CH*Me*$_2$), 20.0 (s, CH*Me*$_2$), 31.3 (C*Me*$_3$), 56.7 (*C*Me$_3$), 127.8, 128.3, 128.3, 128.5, 128.9, 130.0, 131.6, 132.8, 135.8, 137.7, 139.6, 147.9 (d, J_{CF}= 241 Hz, *C*-F) (*Ph*), 177.4 (N*C*N); **^{11}B NMR (160 MHz, C_6D_5Br)**: δ -15.9 (s); ^{19}F{^{1}H} NMR (471 MHz, C_6D_5Br): δ -131.4 (m, 2F, o-*F*) , -161.8 (t, J_{FF} = 23.55 Hz, 1F, m-*F*), -165.6 (m, 2F, p-*F*); **^{29}Si NMR (100 MHz, C_6D_5Br)**: δ 7.7 (*i*Pr$_3$*Si*–Si), 37.6 (*i*Pr$_3$*Si*–As), 55.1 (*Si*–As). **ATR-IR**: *v* 2360, 2330, 2158, 2023, 1973, 1514, 1462, 1355, 1082, 977, 756, 682, 661.

II. Spectroscopic Characterization

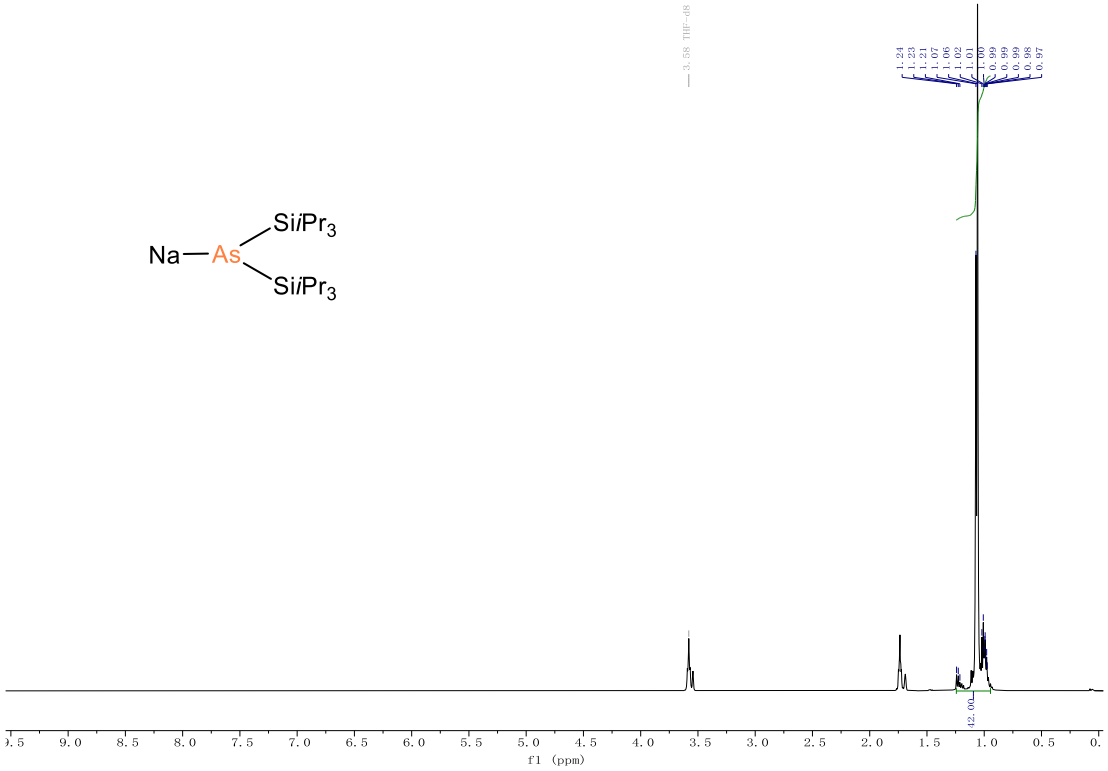


Figure S1. The ^{1}H NMR spectrum of **1** in THF-d_8 at 298K.

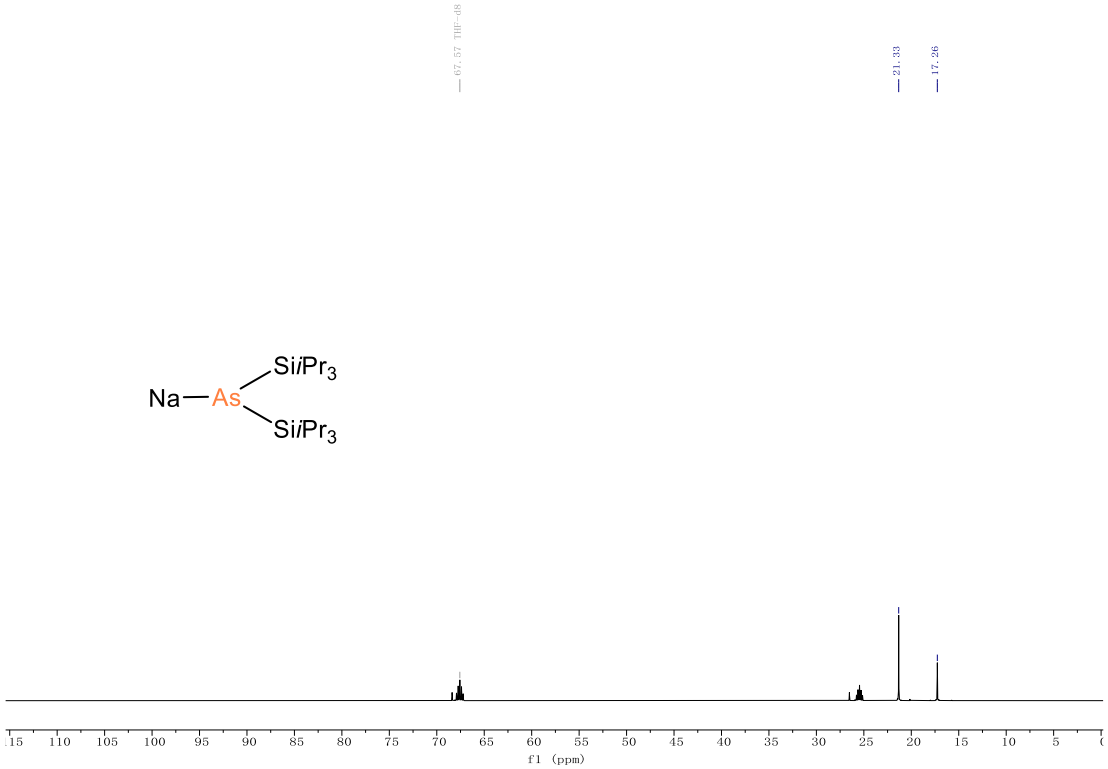


Figure S2. The $^{13}C\{^{1}H\}$ NMR spectrum of **1** in THF-d_8 at 298K.

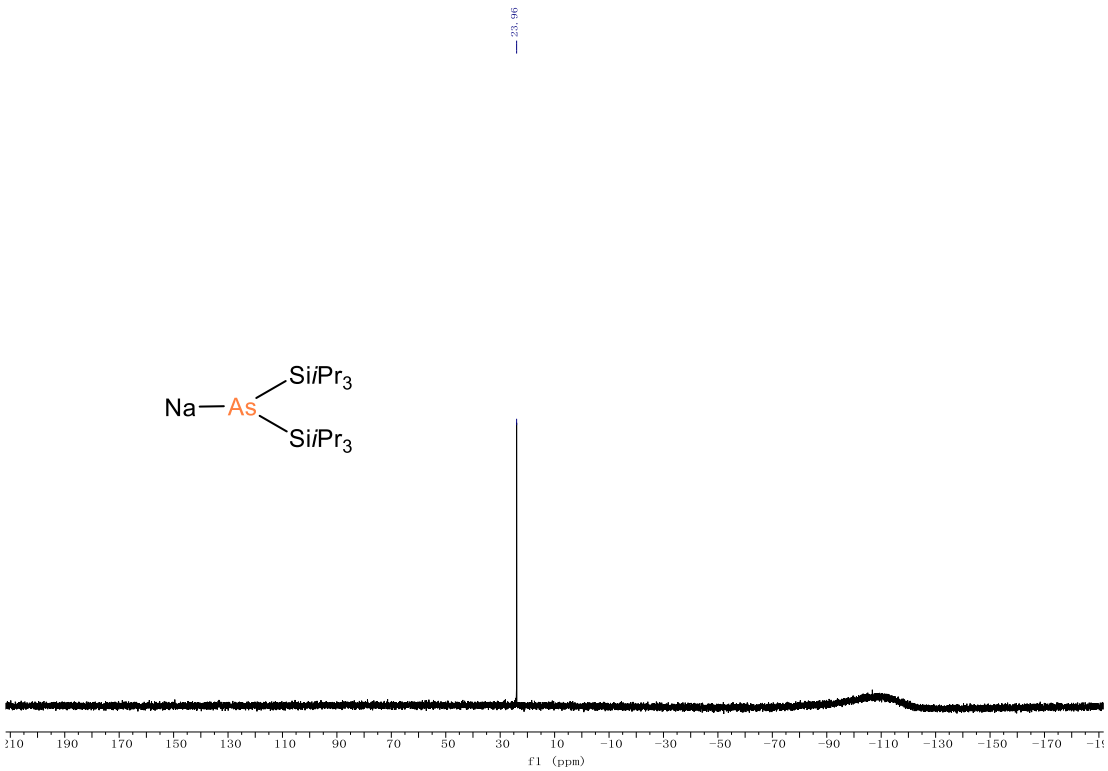


Figure S3. The ^{29}Si NMR spectrum of **1** in THF-d_8 at 298K.

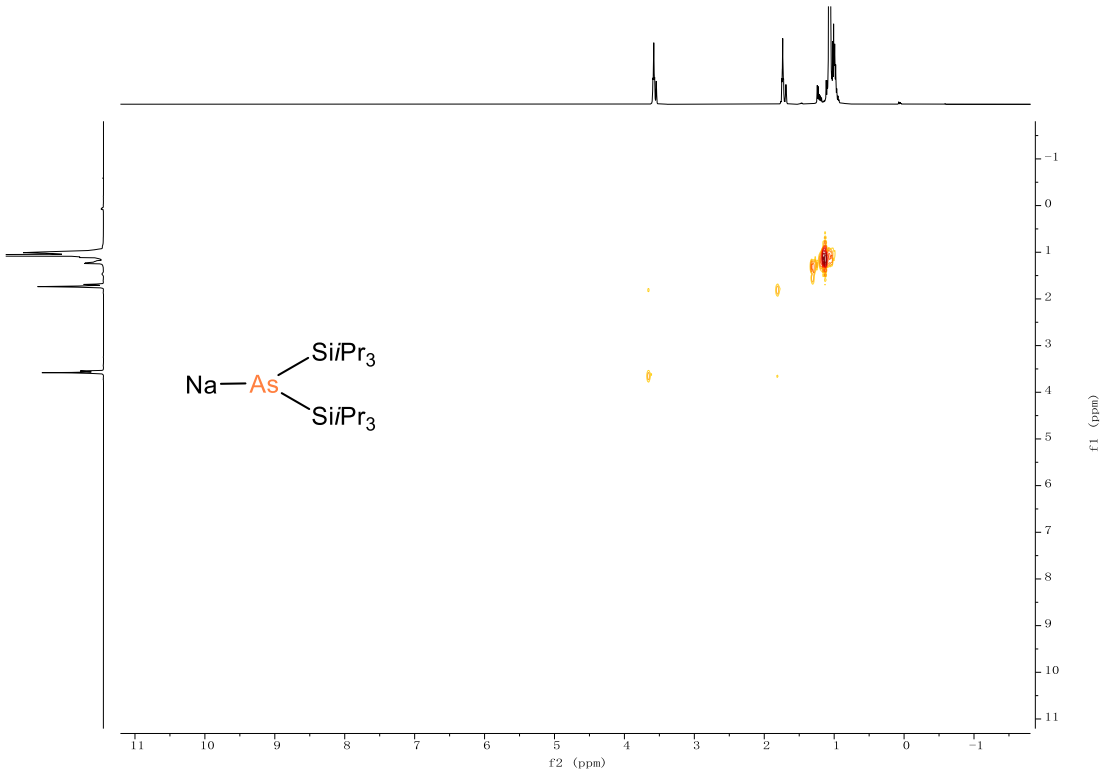


Figure S4. The ^{1}H-^{1}H COSY NMR spectrum of **1** in THF-d_8 at 298K.

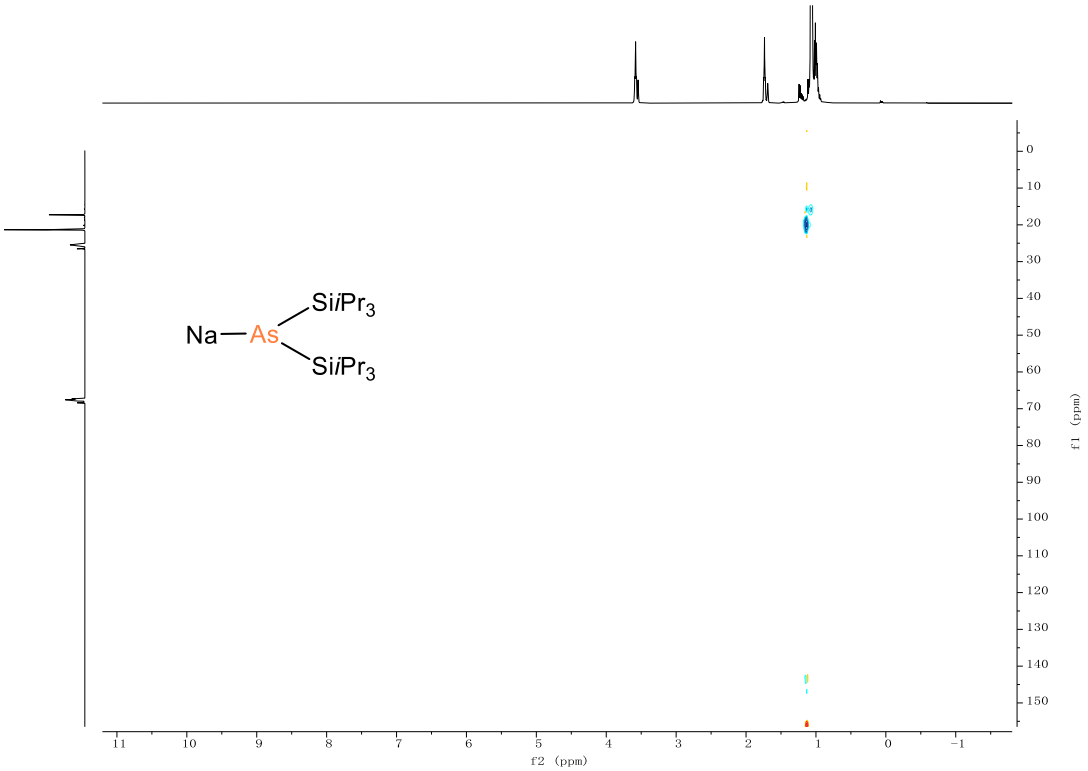


Figure S5. The ^{1}H-^{13}C HSQC NMR spectrum of **1** in THF-d_8 at 298K.

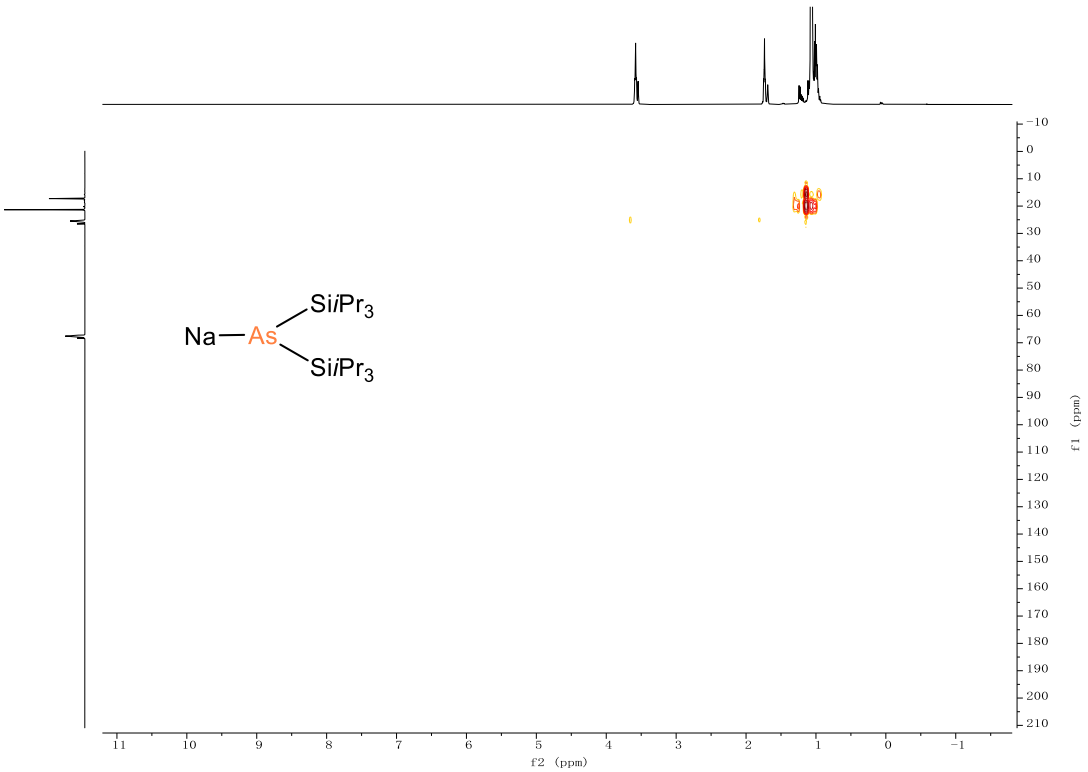


Figure S6. The ^{1}H-^{13}C HMBC NMR spectrum of **1** in THF-d_8 at 298K.

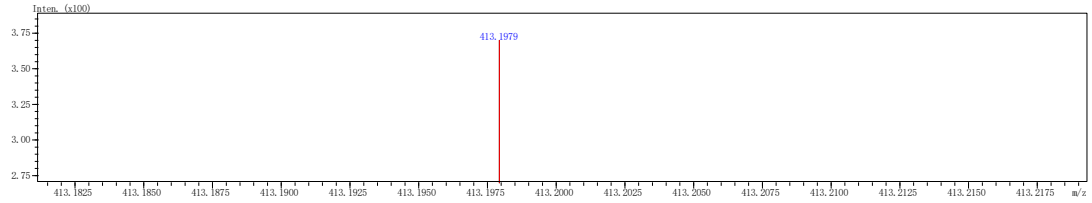


Figure S7. HRMS of **1**.

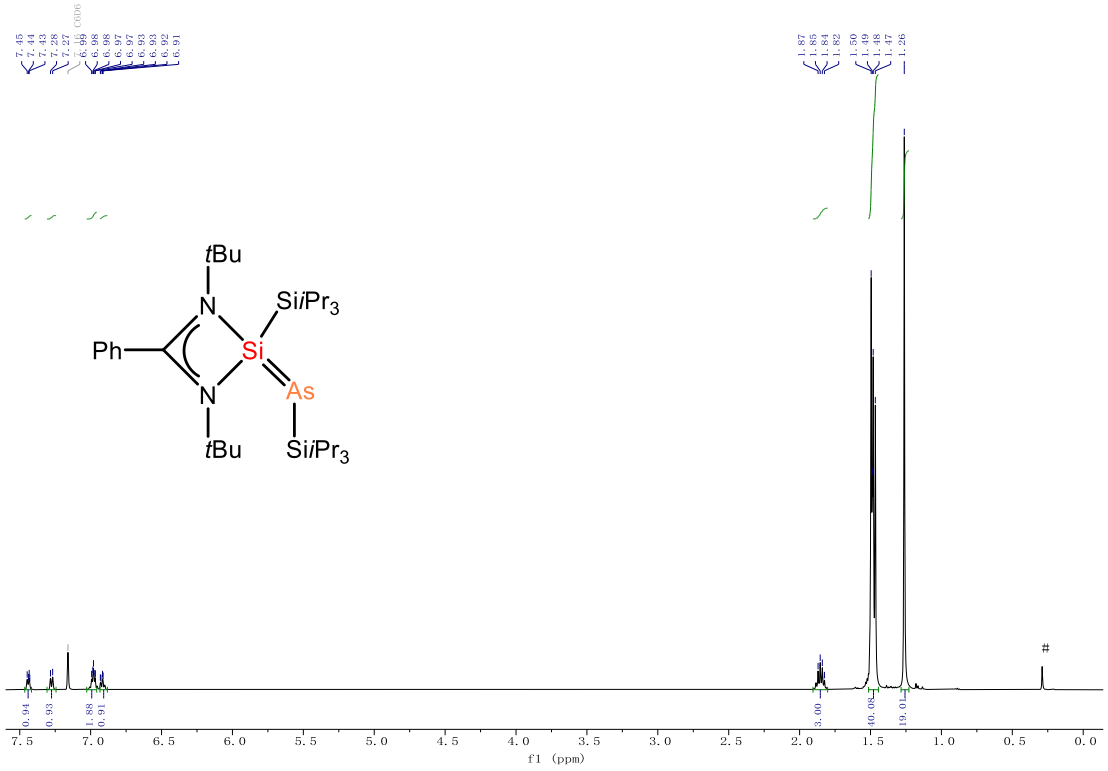


Figure S8. The ^{1}H NMR spectrum of **2** in C_6D_6 at 298K. [#silicon grease]

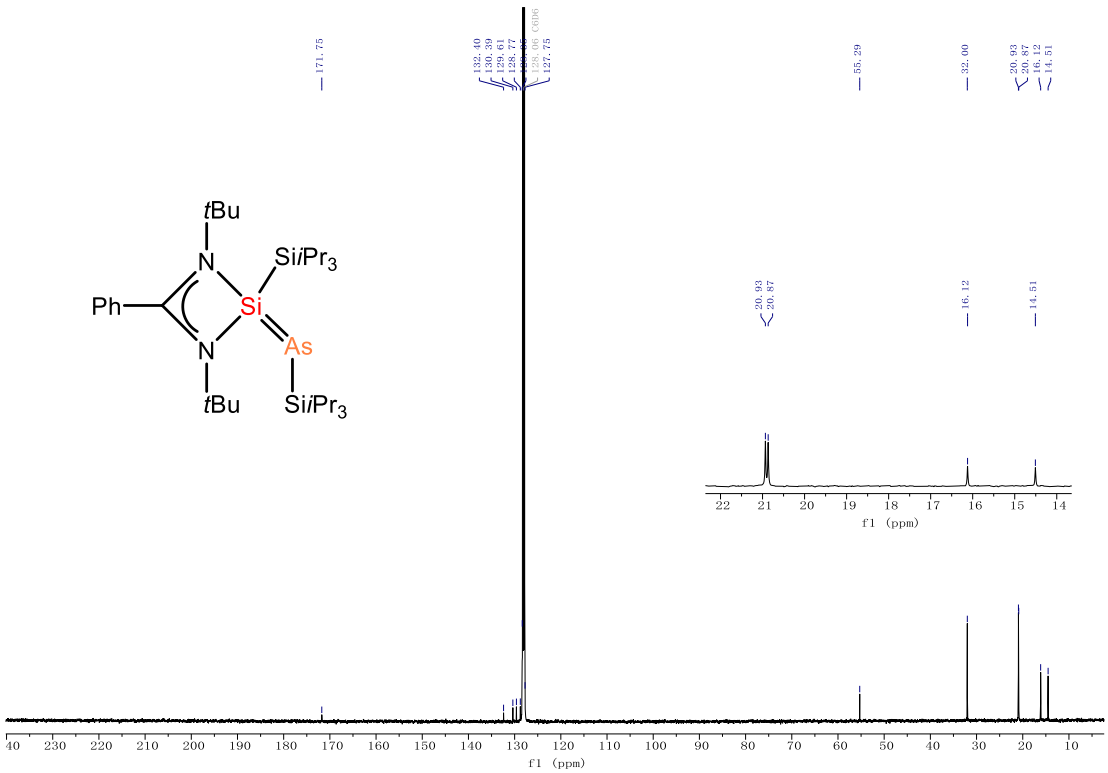


Figure S9. The $^{13}C\{^{1}H\}$ NMR spectrum of **2** in C_6D_6 at 298K.

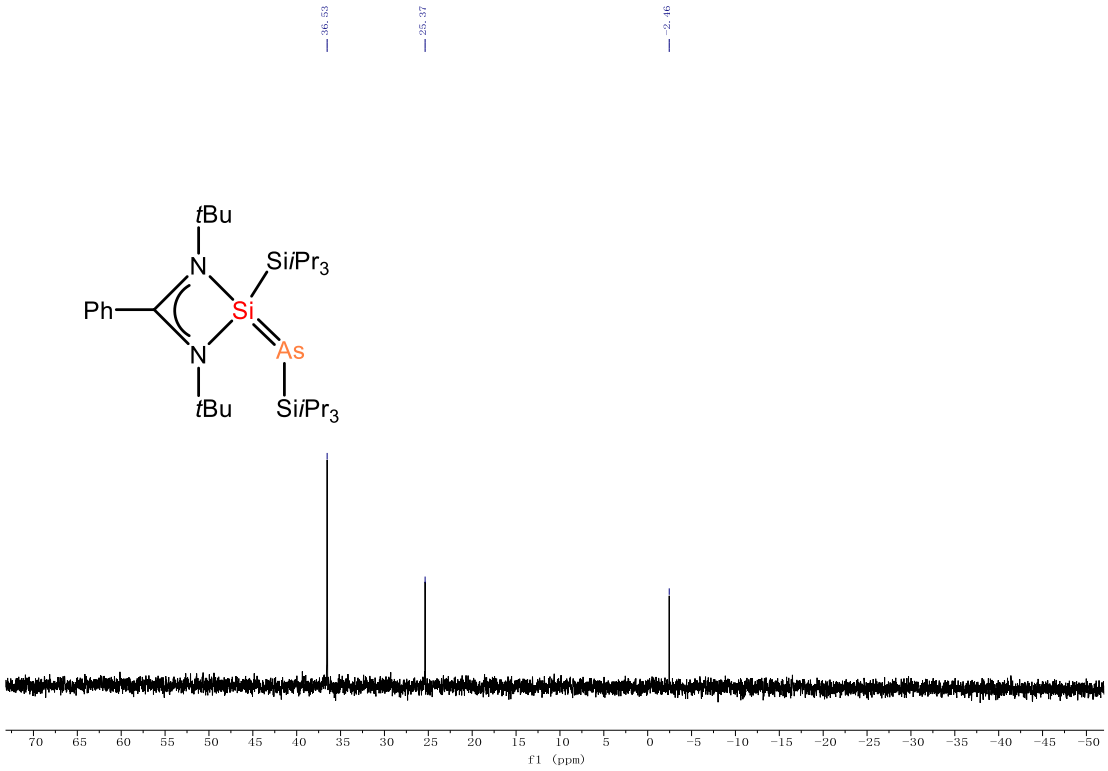


Figure S10. The ^{29}Si NMR spectrum of **2** in C_6D_6 at 298K.

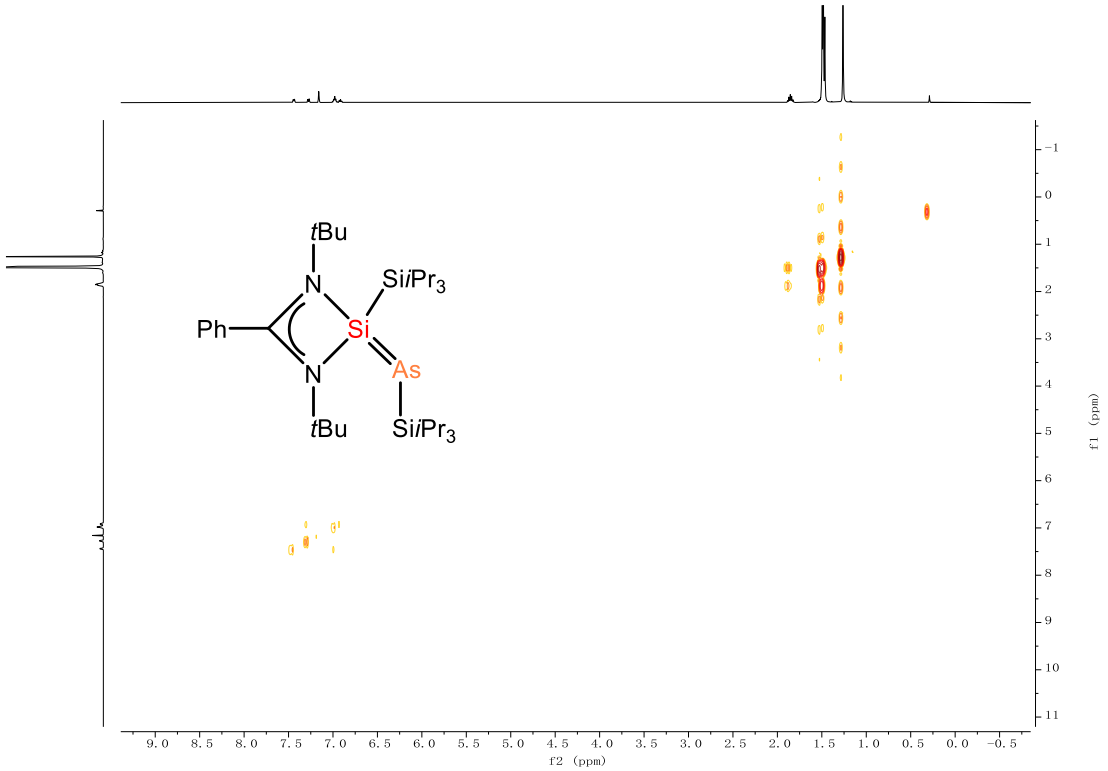


Figure S11. The ^{1}H-^{1}H COSY NMR spectrum of **2** in C_6D_6 at 298K.

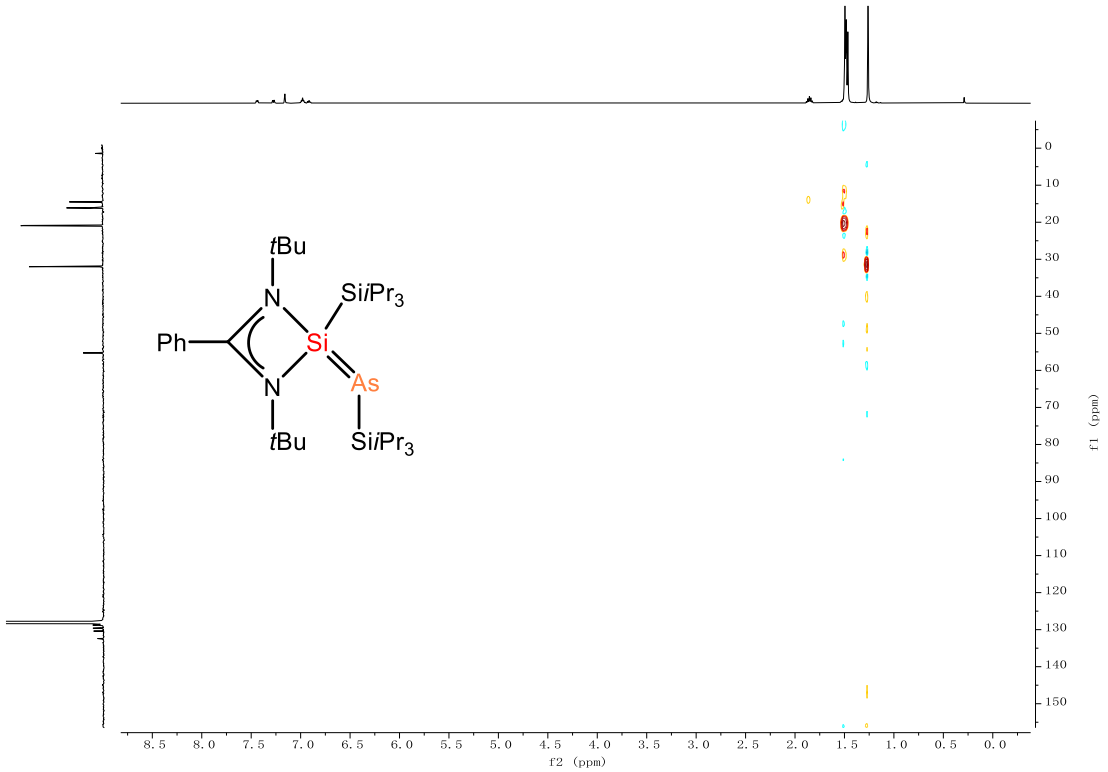


Figure S12. The ^{1}H-^{13}C HSQC NMR spectrum of **2** in C_6D_6 at 298K.

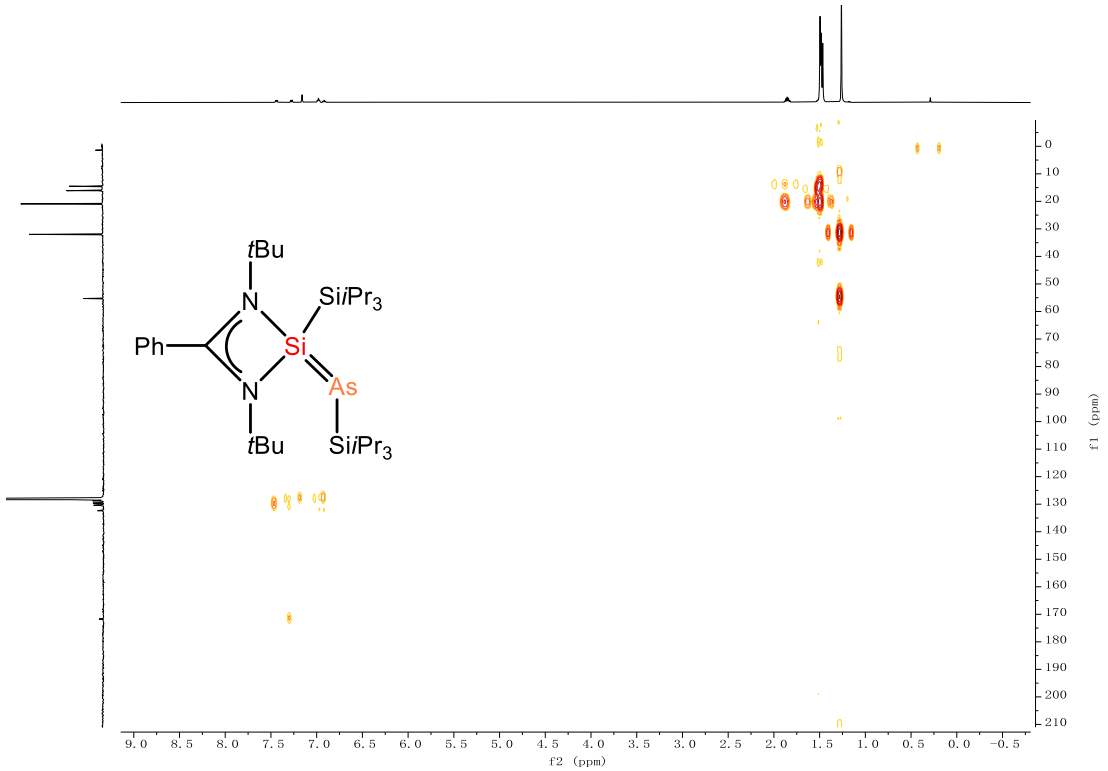


Figure S13. The ^{1}H-^{13}C HMBC NMR spectrum of **2** in C_6D_6 at 298K.

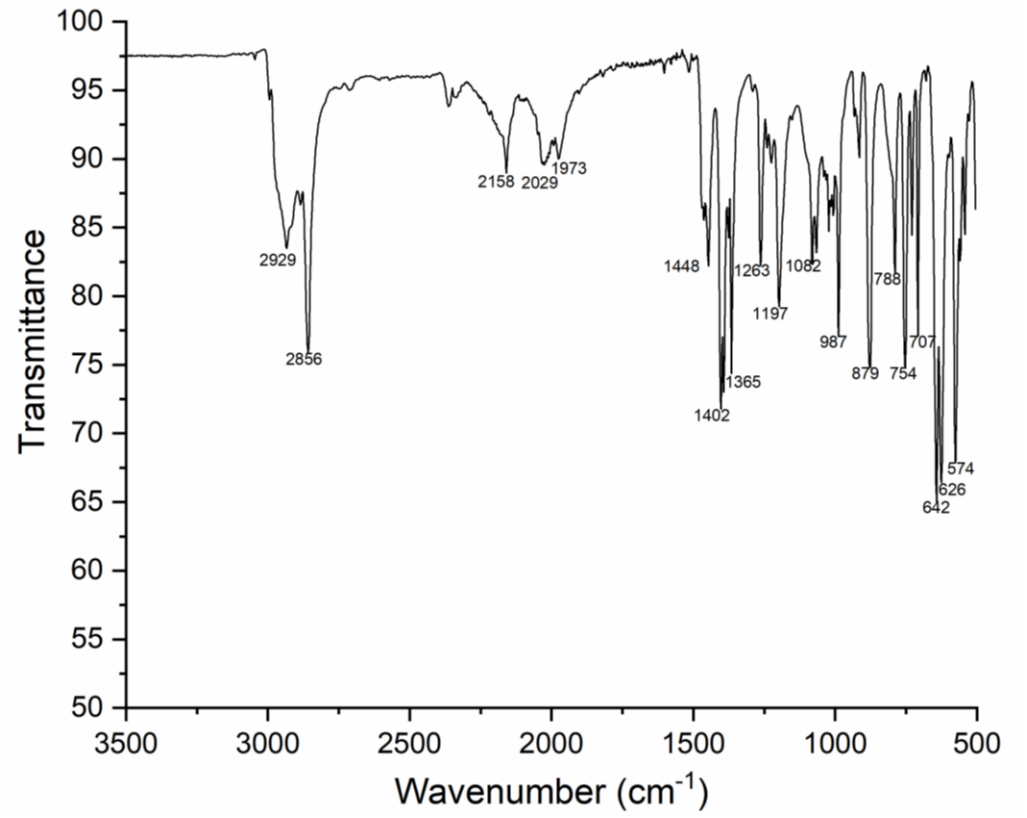


Figure S14. ATR-IR spectrum of **2** in solid form.

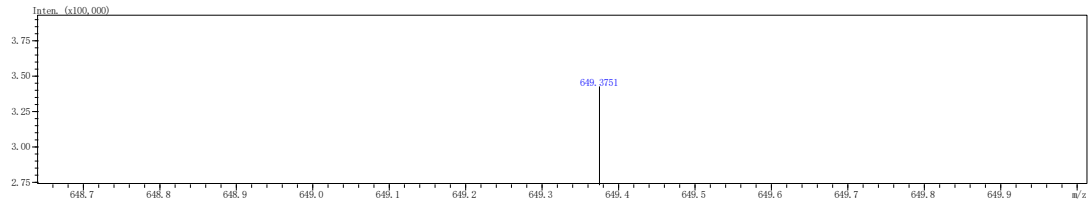


Figure S15. HRMS of **2**.

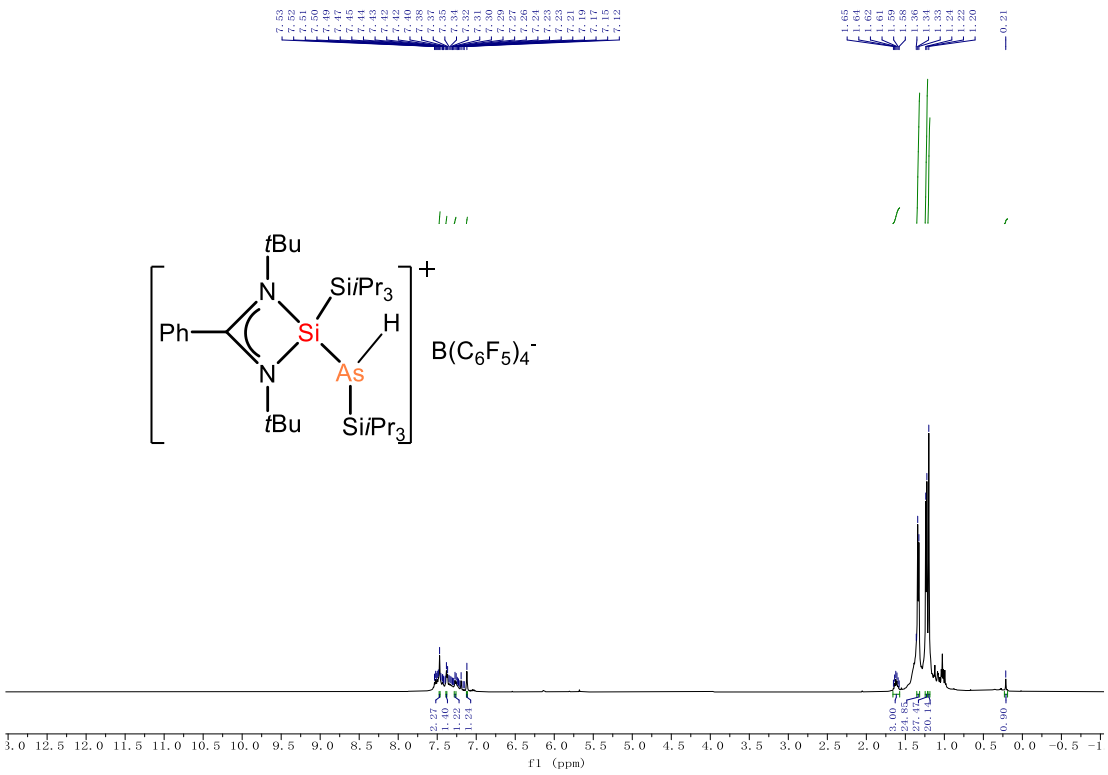


Figure S16. The ^{1}H NMR spectrum of **3** in C_6D_5Br at 298K.

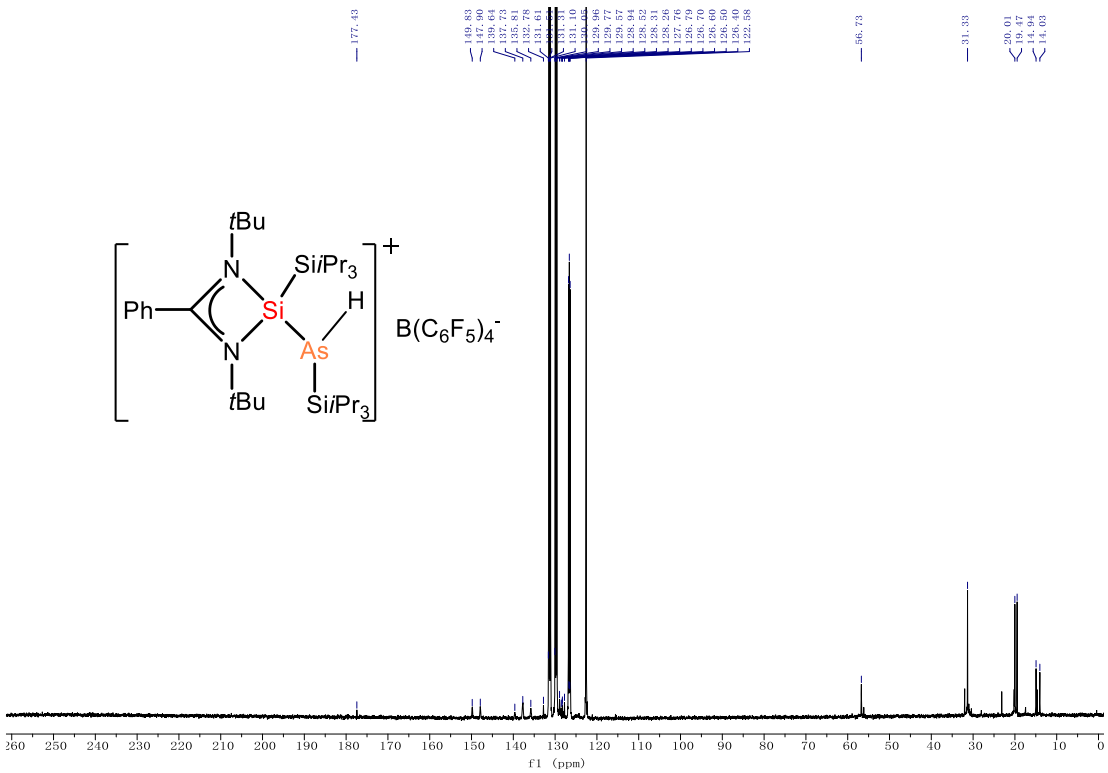


Figure S17. The $^{13}C\{^{1}H\}$ NMR spectrum of **3** in C_6D_5Br at 298K.

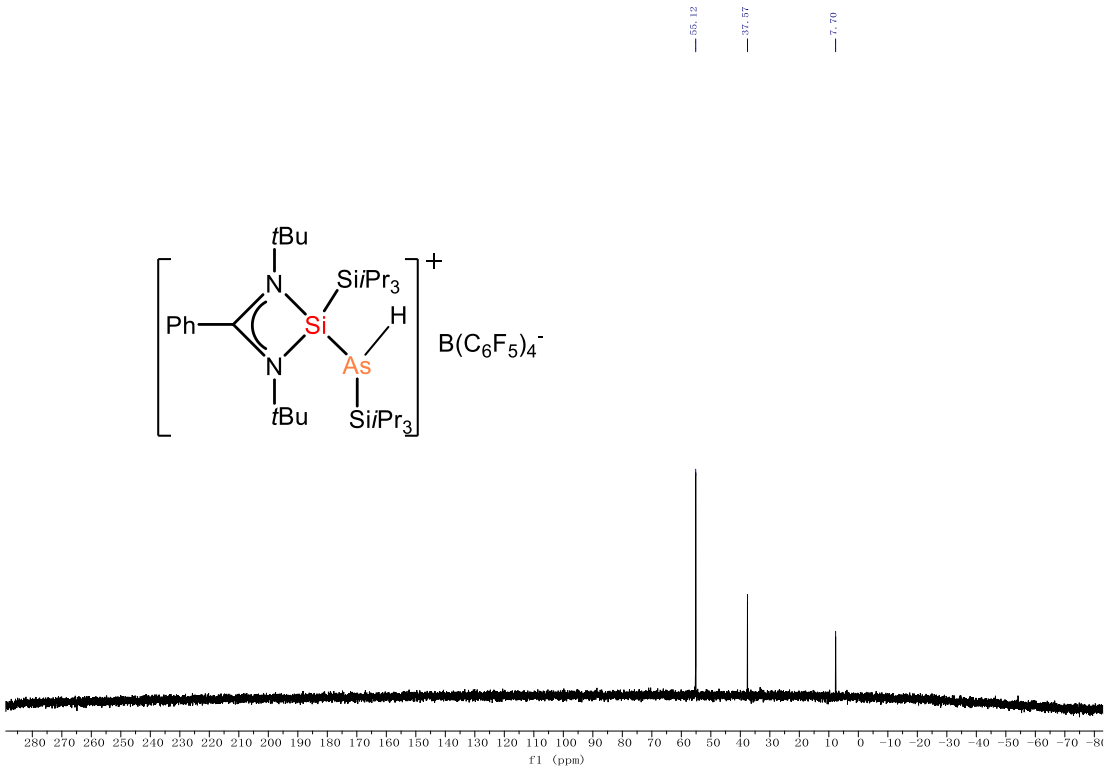


Figure S18. The ^{29}Si NMR spectrum of **3** in C_6D_5Br at 298K.

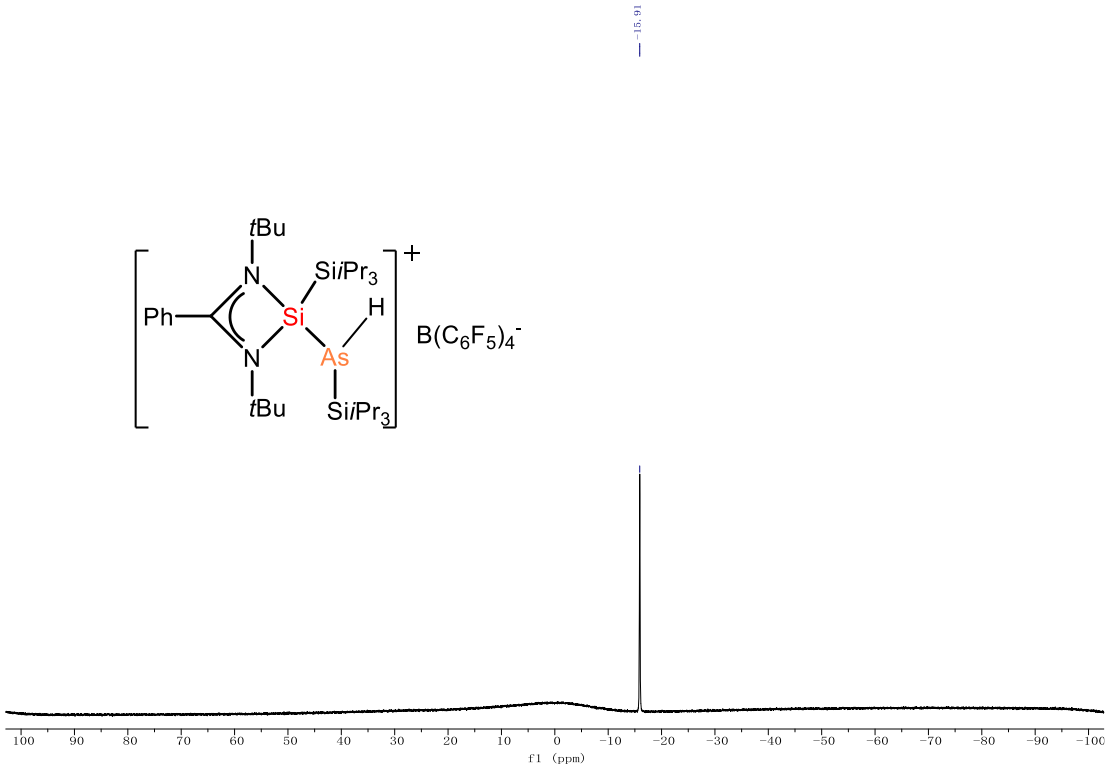


Figure S19. The ^{11}B NMR spectrum of **3** in C_6D_5Br at 298K.

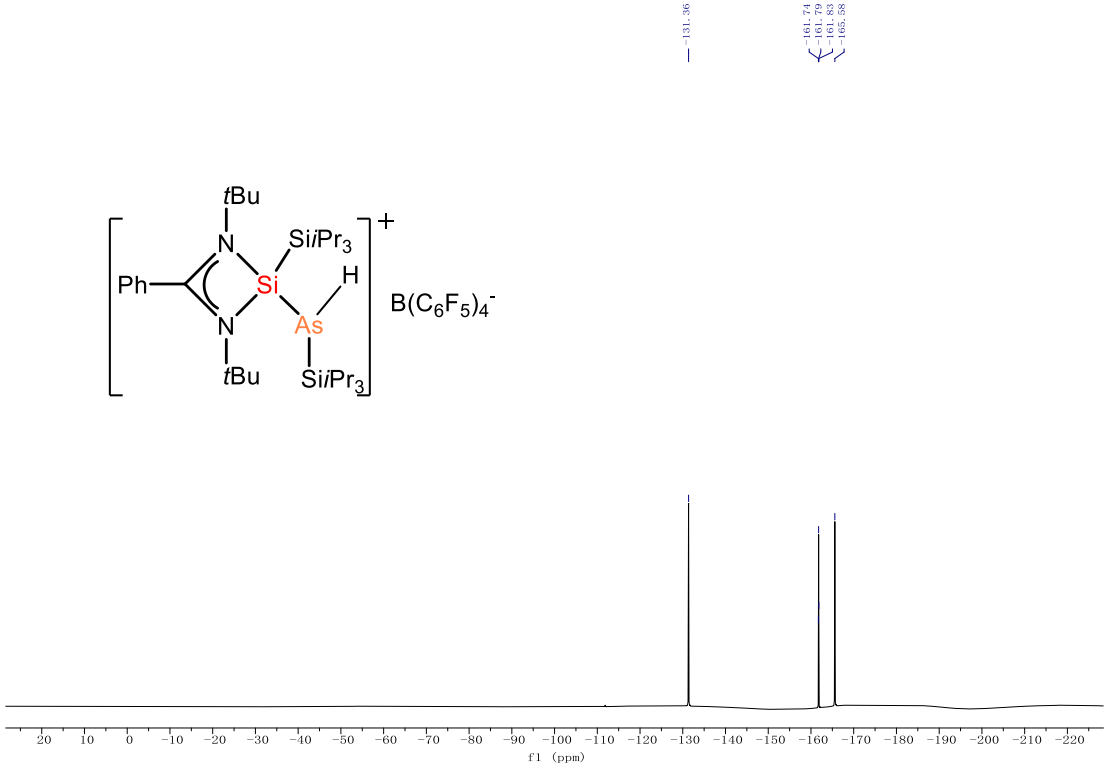


Figure S20. The ^{19}F NMR spectrum of **3** in C_6D_5Br at 298K.

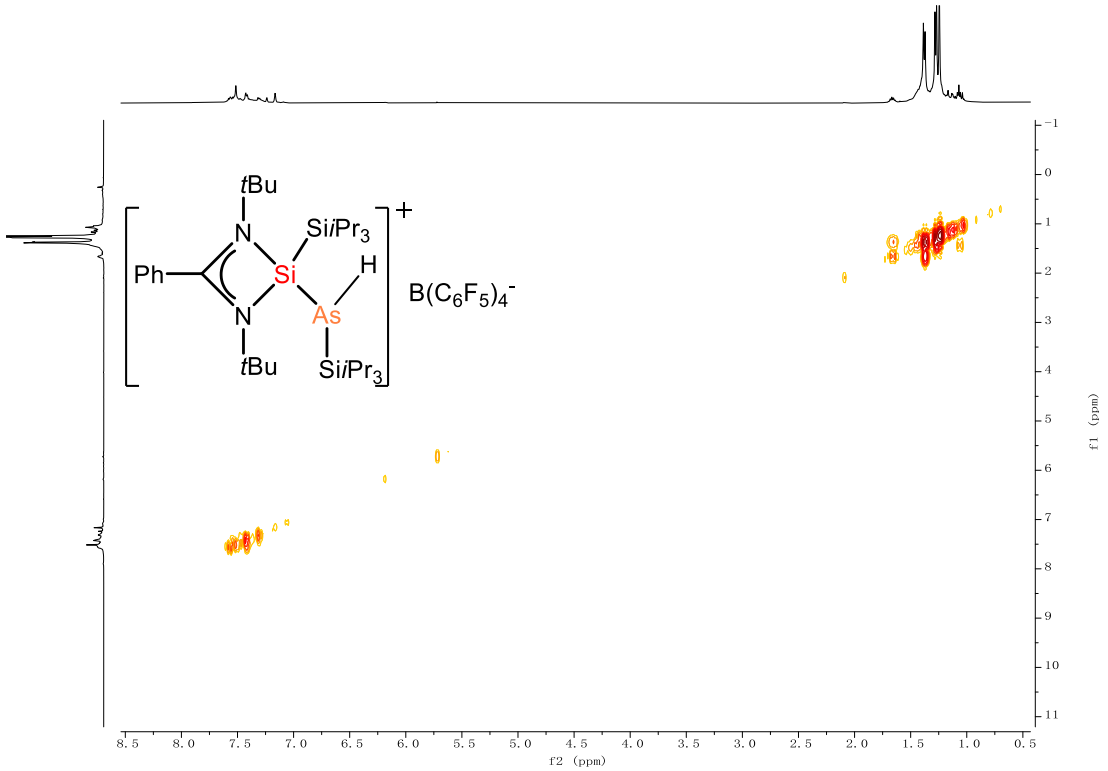


Figure S21. The ^{1}H-^{1}H COSY NMR spectrum of **3** in C_6D_5Br at 298K.

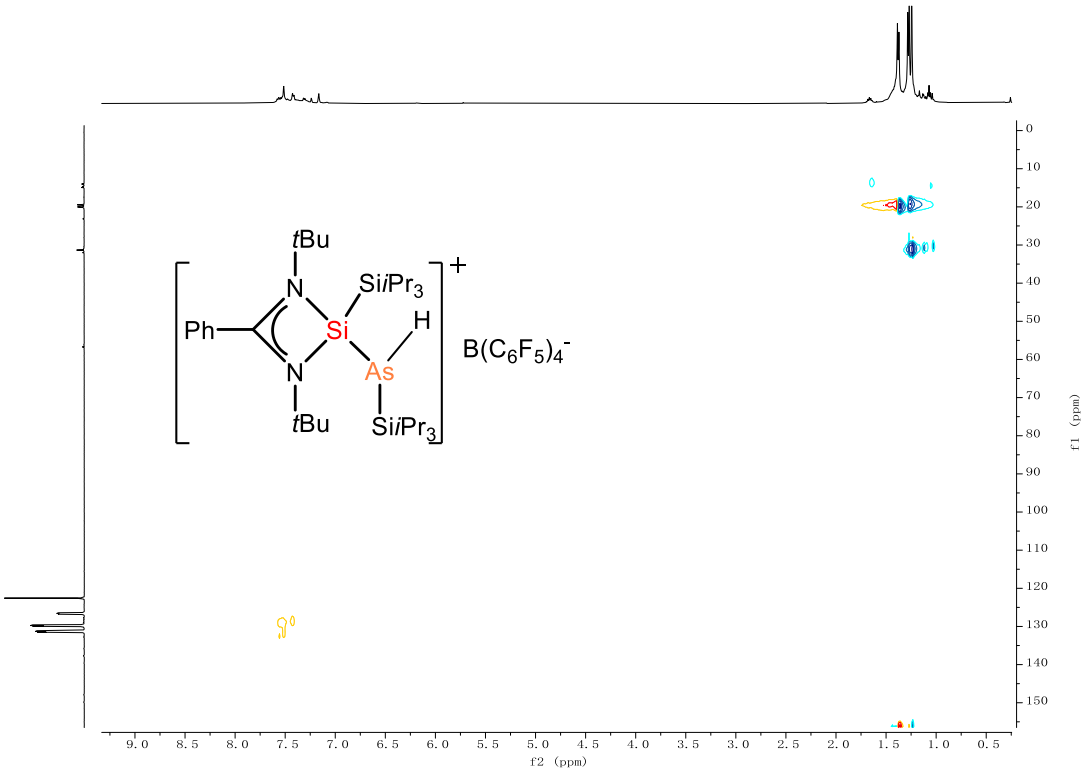


Figure S22. The ^{1}H-^{13}C HSQC NMR spectrum of **3** in C_6D_5Br at 298K.

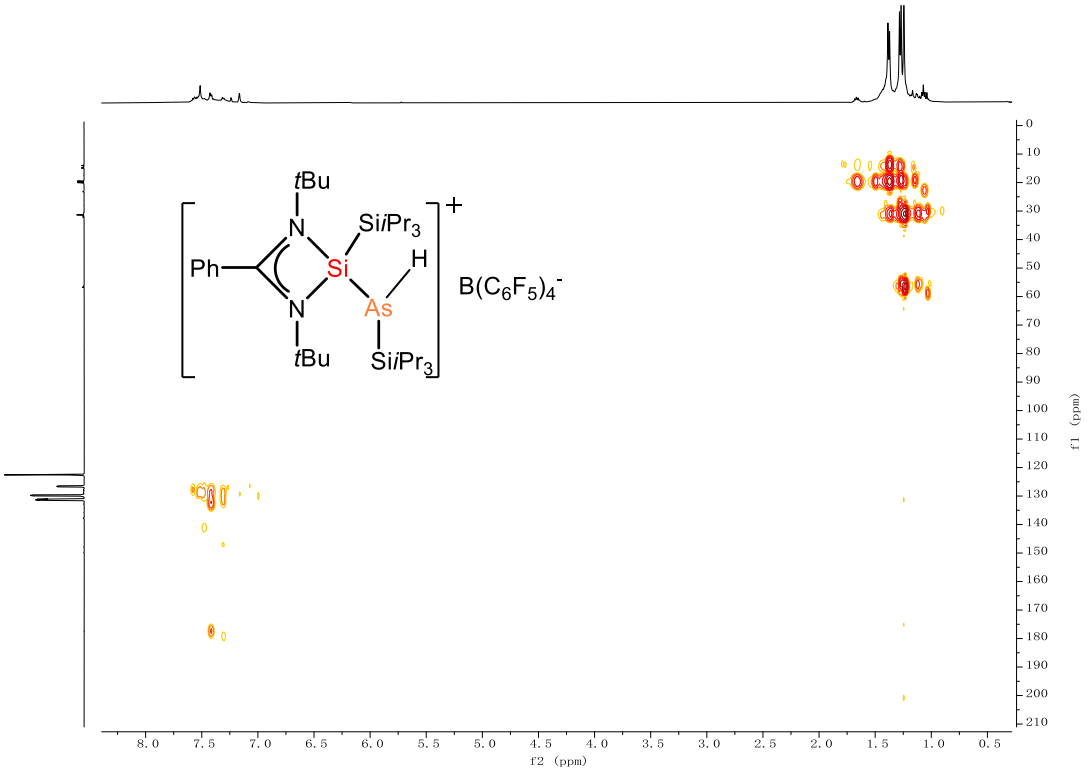


Figure S23. The ^{1}H-^{13}C HMBC NMR spectrum of **3** in C_6D_5Br at 298K.

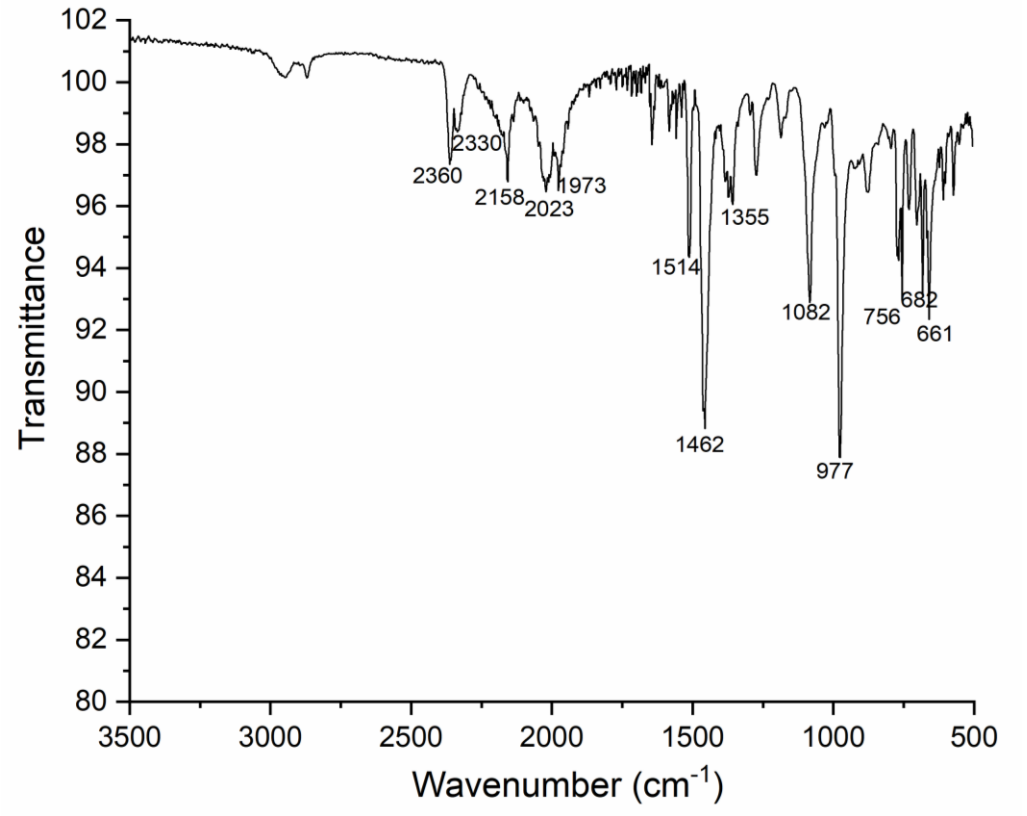


Figure S24. ATR-IR spectrum of **3** in solid form.

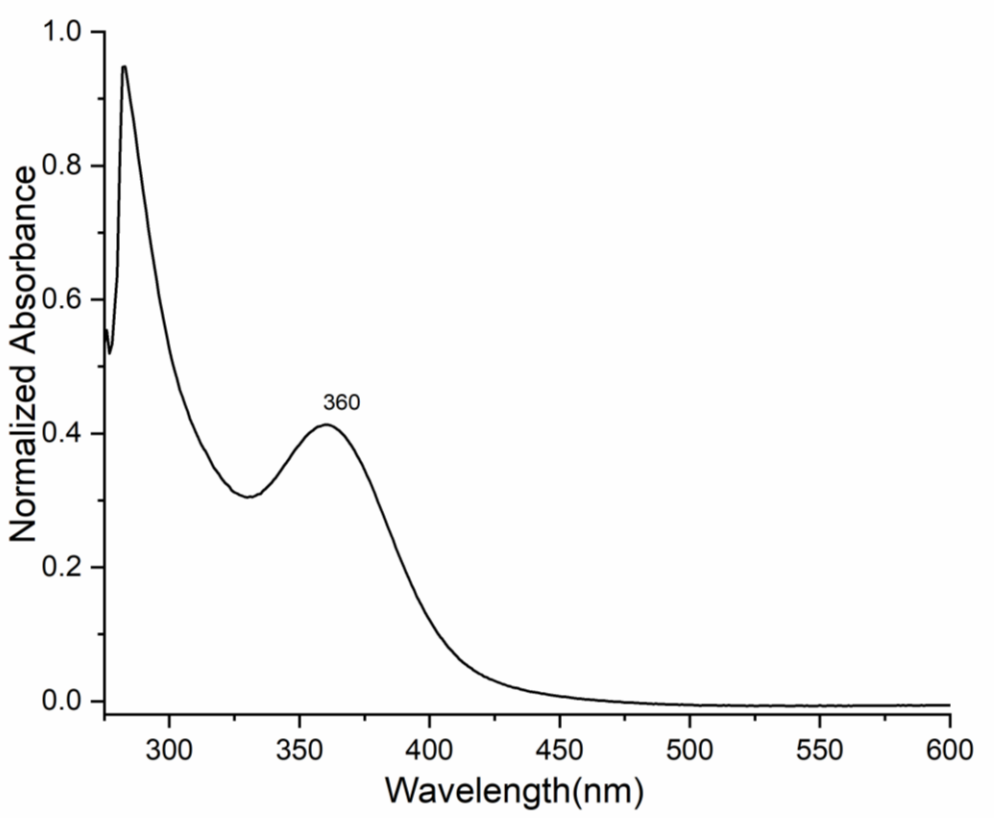


Figure S25. UV-Vis absorption spectrum of **2** in fluorobenzene at 0.05 mM.

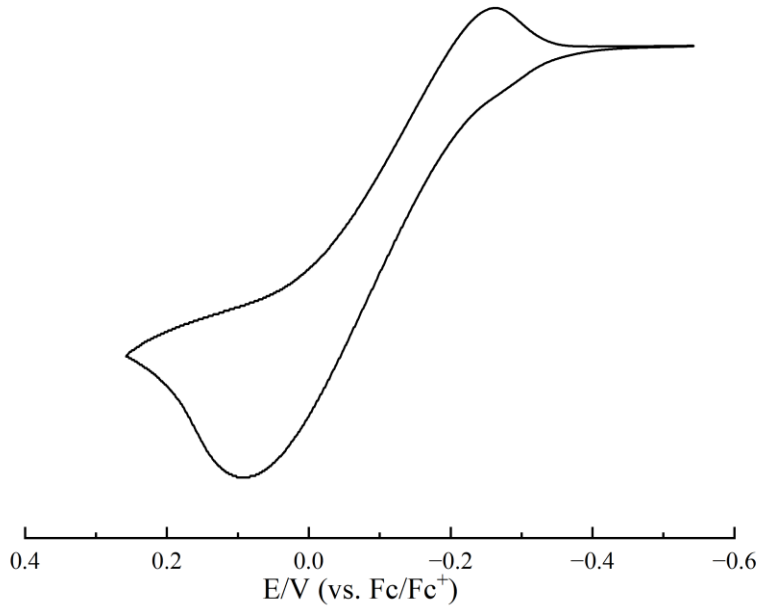


Figure S26. Cyclic voltammograms of **2** in CH_2Cl_2 containing [*n*-Bu_4N][B(3,5-$(CF_3)_2$-$C_6H_3)_4$] (50 mM) as electrolyte at 50 mV s^{-1} scan rate.

III. Crystallographic Details

All crystals were selected and mounted on a suitable support on a Bruker APX-II diffractometer (monochromated CuKα radiation, λ = 1.54178 Å.) Absorption corrections were applied using the spherical harmonics program (multi-scan type). The crystal was kept at a steady *T* = 150 K during data collection. The structure was solved with the ShelXT 2014/5[S2] structure solution program using the Intrinsic Phasing solution method and by using Olex2 1.5[S3] as the graphical interface. The model was refined with version 2017 of ShelXL 2019/3[S4] using Least Squares minimisation. Absorption corrections were performed semi-empirically from equivalent reflections on the basis of multi-scans (Bruker AXS APEX3). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model. In **1**, a half moiety was disclosed, and the whole molecule was obtained by symmetric operation. For **2**, the final refinement was done with a solvent free dataset from a PLATON/SQUEEZE[S5] run. The crystal of **3** contains two independent molecules in asymmetric unit.

Table S1. Crystal and structure refinement data of compounds **1**-**3**.

Compound	(**1**·THF)$_2$	**2**	**3**
Emp. formula	$C_{44}H_{100}As_2Na_2O_2Si_4$	$C_{33}H_{65}AsN_2Si_3$	$C_{57}H_{66}AsBF_{20}N_2Si_3$
Formula weight	969.41	1013.36	1329.115
Temperature [K]	150.00	150.00	150.00
Crystal system	monoclinic	triclinic	triclinic
Space group	*C*2/*c*	*P*-1	*P*-1
a [Å]	13.1747(2)	11.6782(3)	11.8541(3)
b [Å]	18.1470(3)	12.0098(3)	21.8293(6)
c [Å]	23.8700(5)	16.4151(5)	23.7012(6)
α [°]	90	96.868(2)	87.5220(10)
β [°]	101.1080(10)	108.052(2)	89.0510(10)
γ [°]	90	113.9550(10)	88.9880(10)
V [Å^3]	5599.96(17)	1918.95(9)	6125.6(3)
Z	4	2	2
ρ [Mgm^{-3}]	1.150	2.346	1.441
μ [mm^{-1}]	2.669	13.704	2.202
F (000)	2096.0	1261.0	2728.0
Crystal size [mm]	0.15 × 0.1 × 0.1	0.188 × 0.089 × 0.052	0.15 × 0.1 × 0.05
Radiation	CuKα (λ = 1.54178)	CuKα (λ = 1.54178)	CuKα (λ = 1.54178)
θ max [°]	68.23	68.351	68.397
Index ranges	-15 ≤ h ≤ 15, -21 ≤ k ≤ 19, -28 ≤ l ≤ 28	-14 ≤ h ≤ 14, -13 ≤ k ≤ 14, -19 ≤ l ≤ 19	-12 ≤ h ≤ 14, -26 ≤ k ≤ 26, -28 ≤ l ≤ 28
Reflections collected	28152	35053	150189
Independent reflections	5137	7031	22416
R_{int}	0.0336	0.0403	0.0641
Data/restraints/ parameters	5137/69/293	7031/0/370	22416/50/1605
Goodness-of-fit on F^2	1.043	1.054	1.046
*R*1 [$I>2\sigma(I)$]	0.0243	0.0373	0.0444
*wR*2 [$I>2\sigma(I)$]	0.0618	0.0967	0.1173
*R*1 [all data]	0.0262	0.0418	0.0494
*wR*2 [all data]	0.0630	0.0994	0.1208
Largest diff. peak and hole max./min.[e·Å^{-3}]	0.25/-0.24	1.65/-0.50	0.74/-0.66

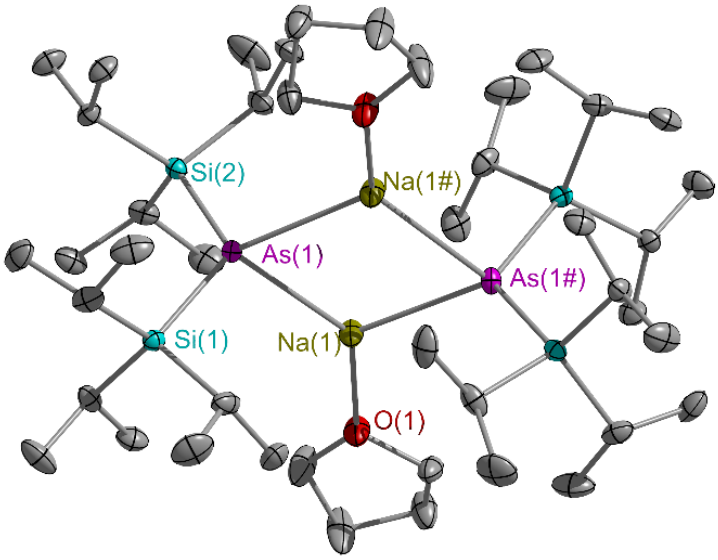


Figure S27. Molecular structure of **1** with thermal ellipsoids presented at the 30% probability level. All hydrogen atoms have been omitted for clarity. Selected bond length (Å) and angels (°): As(1)-Si(1) 2.3214(4), As(1)-Si(2) 2.3228(4), As(1)-Na(1) 2.8762(6), Na(1)-O(1) 2.2484(13); Si(1)-As(1)-Si(2) 118.490(15), Si(1)-As(1)-Na(1) 108.156(18), Si(2)-As(1)-Na(1) 106.998(18), O(1)-Na(1)-As(1) 136.10(4).

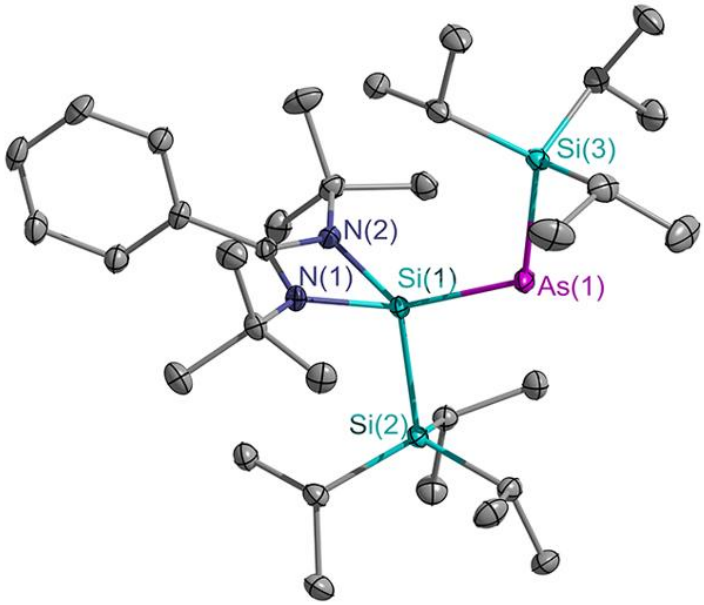


Figure S28. Molecular structure of **2** with thermal ellipsoids presented at the 30% probability level. All hydrogen atoms have been omitted for clarity. Selected bond length (Å) and angels (°): As(1)-Si(1) 2.2111(6), As(1)-Si(3) 2.3358(6), Si(1)-Si(2) 2.4095(8), Si(1)-N(1) 1.8652(18), Si(1)-N(2) 1.8695(18); Si(1)-As(1)-Si(3) 116.90(2), As(1)-Si(1)-Si(2) 104.18(3), N(1)-Si(1)-As(1) 126.60(6), N(1)-Si(1)-Si(2) 112.33(6), N(1)-Si(1)-N(2) 70.13(8), N(2)-Si(1)-As(1) 128.12(6), N(2)-Si(1)-Si(2) 112.80(6).

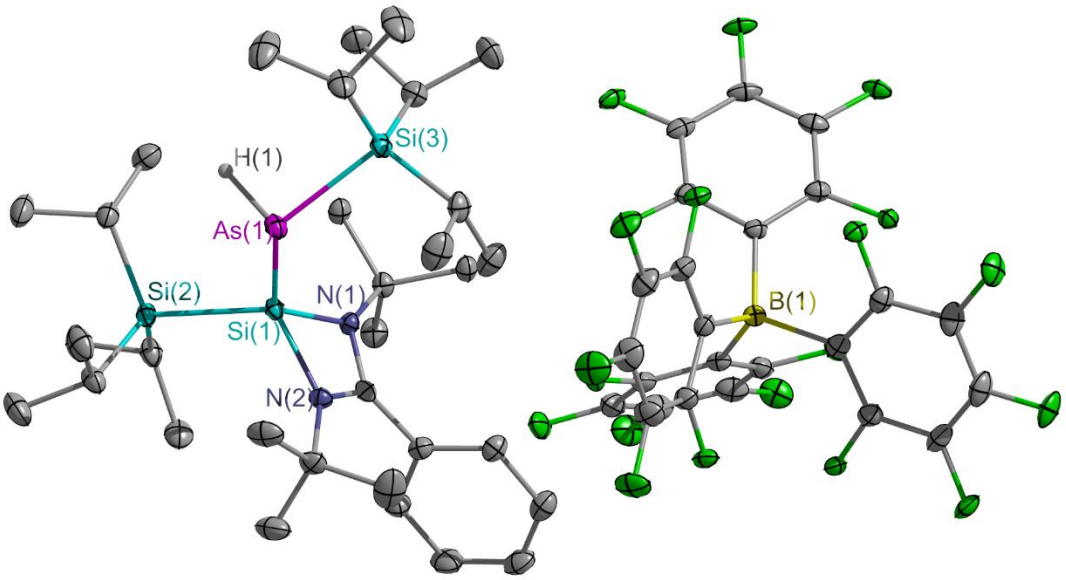


Figure S29. Molecular structure of **3** with thermal ellipsoids presented at the 30% probability level. All hydrogen atoms have been omitted for clarity. Selected bond length (Å) and angels (°): As(1)-Si(1) 2.3195(6), As(1)-Si(3) 2.3885(7), Si(1)-Si(2) 2.4165(8), Si(1)-N(1) 1.8210(18), Si(1)-N(2) 1.8254(19); Si(1)-As(1)-Si(3) 121.38(2), As(1)-Si(1)-Si(2) 107.41(3), N(1)-Si(1)-As(1) 127.11(6), N(1)-Si(1)-Si(2) 116.92(6), N(1)-Si(1)-N(2) 72.00(8), N(2)-Si(1)-As(1) 112.17(6), N(2)-Si(1)-Si(2) 117.08(7).

IV. Computational Details

General computational methods: Geometry optimizations were carried out with the Gaussian 16 package[S6] with the M06-2X functional.[S7] The def2-SVP 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). All the 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 7.0 program [S8] at the M06-2X/def2-TZVP level of theory. Optimized structures were visualized by the Chemcraft,[S9] and IBOview [S10] programs. Intrinsic bond orbitals (IBOs) were carried out using ORCA program [S11] at the M06-2X-D3/def2-SVP level of theory.

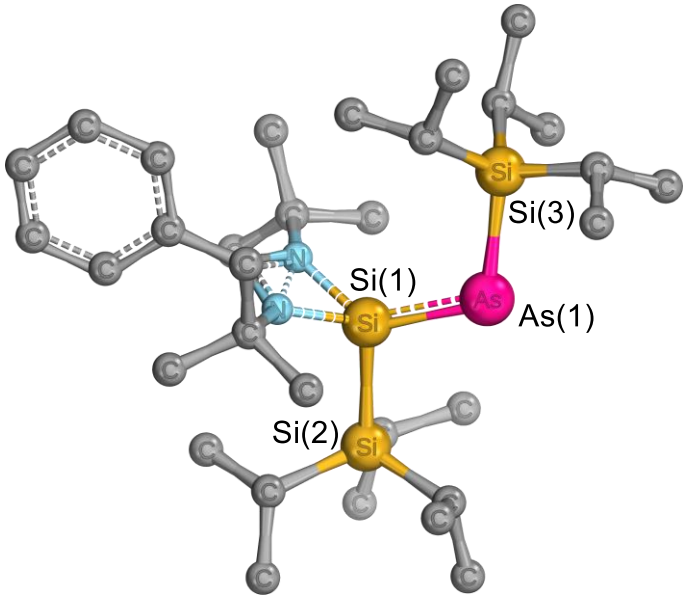


Figure S30. The optimized structure of **2** (M06-2X/def2-SVP level); Hydrogen atoms are omitted for clarity.

Table S2. Selected bond length (Å) and angles (°) of the crystal structure and the optimized structure of **2**.

	Crystal structure of **2**	DFT optimized structure of **2**
As(1)−Si(1)	2.2111(6)	2.22129
As(1)−Si(3)	2.3358(6)	2.35256
Si(1)−Si(2)	2.4094(8)	2.39036
Si(1)−As(1)−Si(3)	116.90(2)	110.664
Si(2)−Si(1)−As(1)	104.18(3)	106.886

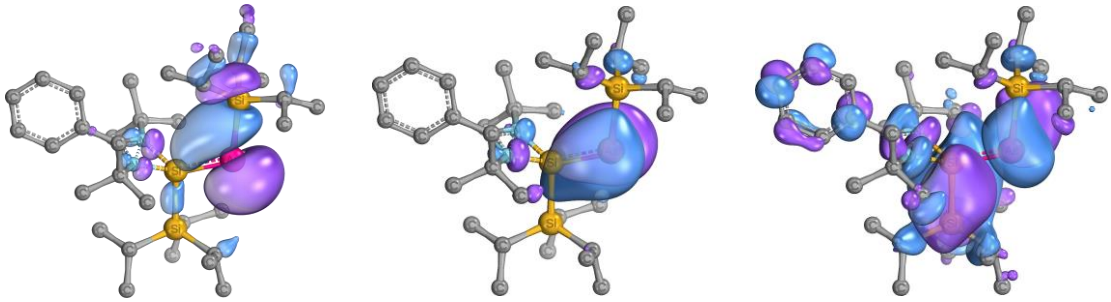


Figure S31. Selected molecular orbitals of **2**. Threshold value = 80.

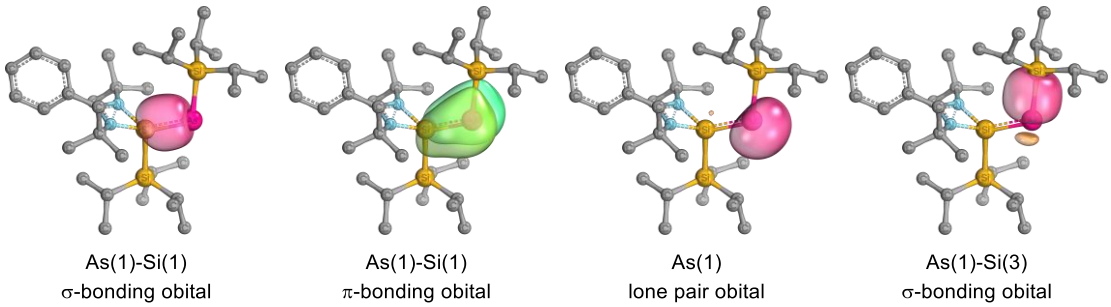


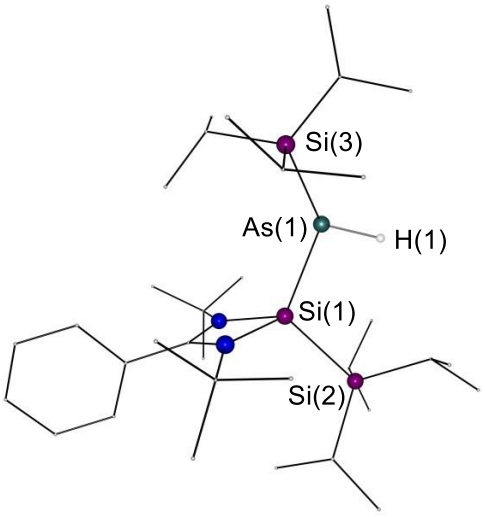
Figure S32. Selected IBOs of **2**. Threshold value = 80.

Table S3. Selected WBI (Wiberg bond index) values of **2**.

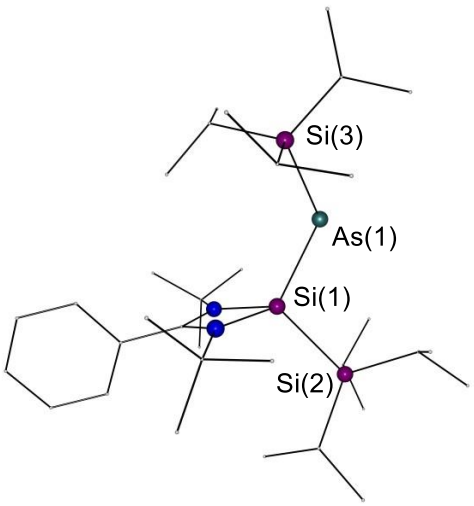
Selected bond	Wiberg bond index
As(1)−Si(1)	1.51
As(1)−Si(3)	0.99
Si(1)−Si(2)	0.90

Table S4. Selected NPA (natural population analysis) charges of **2**.

Selected atom	NPA charge
As(1)	−0.76
Si(1)	+1.05
Si(2)	+1.43
Si(3)	+1.58



The cation of **3**



The hypothetic radical cation

	Crystal structure of **3**	DFT optimized structure of the cation of **3**	DFT optimized structure of the hypothetic radical cation
As(1)−Si(1)	2.3195(6)	2.33933	2.34532
As(1)−Si(3)	2.3885(7)	2.40949	2.41099
Si(1)−Si(2)	2.4165(8)	2.41033	2.40596
Si(1)−As(1)−Si(3)	121.38(2)	113.778	112.424

Figure S33. Structural comparison of the crystal structure (Selected bond length (Å) and angles (°)) of **3** with the optimized structure of **3** and the hypothetic radical cation (M06-2X/def2-SVP level). Hydrogen atoms are omitted for clarity.

IV. References

S1. S. S. Sen, H. W. Roesky, D. Stern, J. Henn and D. Stalke, *J. Am. Chem. Soc.*, 2010, **132**, 1123.

S2. G. Sheldrick, *Acta Crystallogr. C*, 2015, **71**, 3.

S3. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Crystallogr.*, 2009, **42**, 339.

S4. G. Sheldrick, *Acta Crystallogr. A*, 2015, **71**, 3.

S5. P. van der Sluis and A. L. Spek, *Acta Crystallogr. A* 1990, **46**, 194.

S6. M. J. Frisch, M. J. et al. Gaussin 16 rev. B.01 (Gaussian, Inc., Wallingford CT, 2016).

S7. Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc.* 2008, **120**, 215.

S8. E. D. Glendening, J. K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales, P. Karafiloglou, C. R. Landis, F. Weinhold, NBO 7.0, University of Wisconsin: Madison, WI, 2018.

S9. Andrienko, G. A. ChemCraft (http://www.chemcraftprog.com).

S10. G. Knizia, *J. Chem. Theory Comput*. 2013, **9**, 4834.

S11. F. Neese, F. *WIREs Comput. Mol. Sci.*, 2012, **2**, 73.

Cartesian Coordinates:

Compound **2**:

As	-1.62280900	-1.58154800	-0.29282900
Si	0.32596400	-0.53631700	-0.08327900
Si	2.01285400	-2.22670200	0.02066200
Si	-3.40678600	-0.06374300	-0.07320300
N	0.96611000	0.92997600	-1.10677300
N	0.76905400	0.92377500	1.03411300
C	1.16585000	1.65455200	-0.01016600
C	1.74163500	3.03358500	0.04388600
C	1.15305400	1.26888500	-2.52848900
C	3.60421600	-1.51238300	-0.76840600
H	3.25330500	-1.02596900	-1.69551700
C	0.76676800	1.23528400	2.47467900
C	-3.24089100	1.51498700	-1.15529800
H	-2.71949800	1.15366200	-2.05955900
C	-3.64519900	0.47057500	1.75371900
H	-2.76785900	1.11934500	1.94054300
C	2.29294200	-2.65618500	1.86751900
H	2.35640700	-1.67775100	2.37579800
C	3.12204900	3.21617300	0.17951300
H	3.78104500	2.34918100	0.23830700
C	1.35116900	-3.76125100	-0.90442400
H	0.34272600	-3.91424600	-0.47964300
C	0.90312800	4.14913400	-0.05197100
H	-0.17380900	4.00794400	-0.14958300
C	3.59336300	-3.40694700	2.18164500
H	3.65306900	-4.36832300	1.65060200
H	3.65772300	-3.62623600	3.26029100
H	4.48646400	-2.82555500	1.91162200
C	0.00731000	0.10188100	3.16461000
H	-1.02419900	0.04358400	2.79292600
H	-0.01301300	0.27435100	4.24979900
H	0.48714700	-0.86856600	2.97798200
C	2.16393000	-5.03886500	-0.65419100
H	3.21081700	-4.93759700	-0.97873700
H	1.72849800	-5.88014100	-1.21768500
H	2.17127100	-5.32683000	0.40600400
C	2.19812300	1.30275500	3.01949000
H	2.72808200	0.35560600	2.84418300
H	2.17470800	1.48884200	4.10320900
H	2.76639300	2.11660400	2.54800700
C	2.57808600	1.76196900	-2.81036000
H	2.75028400	2.77036400	-2.41184700

H	2.74019500	1.79838800	-3.89742700
H	3.32077300	1.07746700	-2.37308500
C	0.13460300	2.32847900	-2.96212200
H	-0.88795100	1.97031600	-2.77993200
H	0.24753800	2.53192800	-4.03708600
H	0.28362500	3.27286600	-2.42095700
C	3.65586900	4.50264700	0.22193400
H	4.73324100	4.63602700	0.32657100
C	1.07813400	-3.40422100	2.43467900
H	0.12407400	-2.91635300	2.17817500
H	1.14229200	-3.48493800	3.53211700
H	1.02866000	-4.42854700	2.03415700
C	4.17911100	-0.41581600	0.13465300
H	3.39906200	0.28388200	0.47326900
H	4.96497900	0.16346300	-0.38007200
H	4.63303600	-0.84526300	1.04177600
C	-3.58577900	-0.68006200	2.76438400
H	-4.50947700	-1.27641300	2.74013300
H	-3.47881400	-0.29296600	3.79172300
H	-2.74870600	-1.36438700	2.56037900
C	1.44181900	5.43370900	-0.01118600
H	0.78045100	6.29772900	-0.08514200
C	-2.34946600	2.55510200	-0.47757200
H	-2.83760500	2.97242300	0.41933400
H	-2.13038400	3.39914300	-1.15474600
H	-1.39191000	2.11286700	-0.15702700
C	0.89292700	-0.01405200	-3.31885800
H	1.63417900	-0.78710100	-3.07060000
H	0.96058300	0.19257000	-4.39603100
H	-0.10811000	-0.41144500	-3.09276700
C	-4.56633100	2.14297900	-1.60026300
H	-5.18888400	1.43641300	-2.16710500
H	-4.38530400	3.01767400	-2.24745000
H	-5.16293600	2.49174300	-0.74358100
C	1.17604900	-3.51079100	-2.40515900
H	0.44114100	-2.71535200	-2.59162800
H	0.81109300	-4.42075200	-2.90834800
H	2.12714700	-3.22984700	-2.88941700
C	-4.92634300	-1.01922800	-0.73624200
H	-5.76725100	-0.30231700	-0.68968400
C	0.03692400	2.55490800	2.75817400
H	0.61836100	3.42730500	2.43360200
H	-0.13194000	2.64862100	3.84059900
H	-0.94114600	2.56877900	2.25434800

C	2.81770400	5.61283900	0.12622300
H	3.23754600	6.61911500	0.15836900
C	4.67812800	-2.53133800	-1.16191200
H	5.01507300	-3.12625300	-0.29942400
H	5.56431000	-2.02315400	-1.57741500
H	4.31214000	-3.23221900	-1.92566700
C	-4.90862800	1.31113900	1.96882400
H	-4.90674400	2.23128400	1.36641800
H	-5.01232600	1.60831400	3.02578300
H	-5.81351400	0.74129600	1.70082500
C	-5.30091100	-2.24785800	0.09735400
H	-4.44283700	-2.93083800	0.20792700
H	-6.11497600	-2.81386700	-0.38513600
H	-5.64271300	-1.97417400	1.10523600
C	-4.71519800	-1.41605500	-2.20235100
H	-4.44172300	-0.55893400	-2.83714200
H	-5.62818800	-1.86851800	-2.62334400
H	-3.90240800	-2.15395000	-2.28767600

The cation of **3**:

As	-1.66314800	1.11491000	-0.98849900
Si	0.41716600	0.49775900	-0.11448200
Si	1.79321500	2.46081500	0.13567600
Si	-3.49500300	-0.21999000	-0.17119400
N	0.71576300	-0.91544900	1.04690600
N	1.17785500	-0.89238800	-1.05977100
C	1.27645100	-1.62186500	0.05504900
C	1.90371000	-2.96551200	0.16294900
C	0.72290500	-1.17176800	2.51005300
C	0.15429500	0.08550800	3.16629800
H	-0.84662700	0.32533600	2.77704200
H	0.81255000	0.94956300	2.99799700
H	0.06789100	-0.06370300	4.25086100
C	-0.14748800	-2.38182100	2.86586600
H	-0.16150100	-2.50329800	3.95816100
H	0.25628000	-3.30636100	2.43442600
H	-1.18425200	-2.25186600	2.52708700
C	1.09567000	-4.10696700	0.14916400
H	0.01183900	-4.00503500	0.07896700
C	2.15089600	-1.40486500	3.01923400
H	2.82970500	-0.61385700	2.66952500
H	2.54402400	-2.37721100	2.69621600
H	2.14857900	-1.39435400	4.11820200
C	-3.30877400	-0.50647900	1.69392500
H	-2.24212000	-0.77596900	1.77752700

C	0.65832400	3.84426700	0.78160100
H	-0.16829500	3.88785200	0.04947600
C	3.29506000	-3.08814100	0.23972100
H	3.92370900	-2.19617000	0.26960600
C	1.68237100	-5.36923000	0.20276600
H	1.05281900	-6.25929500	0.18441800
C	3.18783000	1.93604400	1.31956900
H	2.67557700	1.45843400	2.17259900
C	2.41110000	2.87900200	-1.62065600
H	2.68763700	1.91478000	-2.07895500
C	-3.37185800	-1.87418600	-1.08942300
H	-4.21815500	-2.47652500	-0.71188900
C	1.59571400	-1.18710500	-2.45407100
C	0.83751800	-0.20439700	-3.34662500
H	-0.24644400	-0.38700300	-3.30438400
H	1.16654300	-0.31989600	-4.38783400
H	1.02404400	0.83847200	-3.04841000
C	3.06984800	-5.49342500	0.27610600
H	3.52663800	-6.48288600	0.31784800
C	4.02592200	3.08900000	1.88689600
H	4.48608500	3.69801400	1.09528300
H	4.84087100	2.69423400	2.51354300
H	3.42334000	3.75733400	2.51754100
C	0.05796900	3.54085800	2.15680600
H	-0.55744000	2.62796200	2.15018700
H	-0.58728000	4.36848700	2.48956600
H	0.84122000	3.41200700	2.92192100
C	3.66942500	3.76007100	-1.63613500
H	3.50758000	4.72155200	-1.12707200
H	3.95654600	3.98643700	-2.67471200
H	4.52878100	3.27040200	-1.15749400
C	1.29679100	3.50458800	-2.47100500
H	0.36694800	2.91335400	-2.46665700
H	1.62176200	3.60834400	-3.51766100
H	1.04135900	4.51184800	-2.10891300
C	3.87439400	-4.35403300	0.29915900
H	4.95857800	-4.44999500	0.36440200
C	-5.03031200	0.75236900	-0.71425500
H	-5.04417000	0.65008400	-1.81349600
C	4.06727000	0.87156100	0.65089500
H	3.47137100	0.04010800	0.23889900
H	4.79071100	0.44816200	1.36613900
H	4.64494500	1.29613700	-0.18464500
C	-3.54471200	0.74536700	2.54284700

H	-2.96063800	1.60963400	2.18795900
H	-3.26837300	0.56248900	3.59355400
H	-4.60619000	1.03636700	2.53443400
C	3.10566800	-0.97545100	-2.60295900
H	3.39898100	0.04274700	-2.31295900
H	3.39849900	-1.13234500	-3.65060300
H	3.66592100	-1.69071300	-1.98587900
C	-2.07292800	-2.59928000	-0.73081000
H	-2.03692100	-3.60008400	-1.19220600
H	-1.94453100	-2.72154800	0.35681000
H	-1.20337700	-2.03366800	-1.10779900
C	-3.52125600	-1.73349800	-2.60668200
H	-2.74054900	-1.07707500	-3.02634100
H	-4.49541000	-1.31151900	-2.89081900
H	-3.42988500	-2.71305000	-3.10109200
C	-4.13069400	-1.69524500	2.20829800
H	-5.21157000	-1.51209600	2.11574100
H	-3.92178100	-1.87360800	3.27533300
H	-3.90419400	-2.62608400	1.66683500
C	1.34100800	5.22086500	0.77312700
H	2.21609600	5.25225800	1.43800300
H	0.63694600	5.99104800	1.12387100
H	1.67304200	5.51553700	-0.23152700
C	-6.29569600	0.08332200	-0.15701900
H	-6.33947200	-0.99383900	-0.38125300
H	-7.19737600	0.54594300	-0.58626600
H	-6.35844400	0.20309000	0.93585800
C	1.23315600	-2.61697600	-2.87245600
H	1.87056600	-3.36857800	-2.39041200
H	1.37680900	-2.70613000	-3.95824300
H	0.18064100	-2.84386300	-2.64980500
C	-5.00626800	2.25023300	-0.39124400
H	-4.93133900	2.43536900	0.69064000
H	-5.93368800	2.72911700	-0.74094300
H	-4.16815400	2.76671400	-0.88212800
H	-1.80383300	2.24418400	0.02248500

The hypothetic radical cation:

As	-1.68990700	1.09225900	-0.99244700
Si	0.40437500	0.49916000	-0.11909200
Si	1.68423100	2.52039300	0.13626200
Si	-3.46343200	-0.31642600	-0.16595900
N	0.74123700	-0.90331200	1.04292700
N	1.21996500	-0.86209400	-1.06064700
C	1.33251200	-1.58947600	0.05361900

C	2.00580300	-2.91018200	0.16247700
C	0.76673400	-1.15265400	2.50767800
C	0.16120400	0.08657900	3.16487500
H	-0.85262600	0.28817300	2.78938200
H	0.78438600	0.97326800	2.98284200
H	0.09529800	-0.06007800	4.25122100
C	-0.06051600	-2.38951700	2.87363300
H	-0.06109400	-2.50907500	3.96622100
H	0.36886400	-3.30151400	2.44018500
H	-1.10393600	-2.29333100	2.54371400
C	1.24071600	-4.08081000	0.15757000
H	0.15328000	-4.01976500	0.09462500
C	2.20543500	-1.33349500	3.00776800
H	2.85261200	-0.51916900	2.65130100
H	2.63128400	-2.29202100	2.68519900
H	2.20999200	-1.31951200	4.10665400
C	-3.25847200	-0.57870000	1.69968500
H	-2.18697700	-0.83027800	1.77626200
C	0.44032700	3.82724900	0.73965600
H	-0.35462500	3.81555500	-0.02921400
C	3.40136000	-2.98018500	0.22945900
H	3.99583400	-2.06480100	0.25268100
C	1.87520900	-5.31997100	0.21026200
H	1.27959000	-6.23319700	0.19843800
C	3.08915700	2.08241100	1.34254700
H	2.59520200	1.58291400	2.19358100
C	2.31123000	2.96821100	-1.61115500
H	2.64522800	2.01970800	-2.06458200
C	-3.30480400	-1.98176700	-1.06561500
H	-4.14097900	-2.58956100	-0.67347600
C	1.64220300	-1.14079600	-2.45551900
C	0.84813600	-0.18158500	-3.34304700
H	-0.22842200	-0.40593800	-3.30040300
H	1.17844300	-0.27919300	-4.38568900
H	0.99999800	0.86569500	-3.03952800
C	3.26683400	-5.39170500	0.27463600
H	3.76057200	-6.36326300	0.31624700
C	3.85686700	3.28256500	1.91125300
H	4.29766900	3.90771600	1.12141300
H	4.68048600	2.93732600	2.55554400
H	3.20878300	3.92399200	2.52446900
C	-0.20611800	3.47834100	2.08239200
H	-0.75722600	2.52558600	2.04100800
H	-0.92461600	4.25722300	2.38100400

H	0.54254600	3.40004200	2.88789700
C	3.52262900	3.91299300	-1.60287800
H	3.30052800	4.86412000	-1.09674400
H	3.81624500	4.15559400	-2.63597500
H	4.39758500	3.46891300	-1.10859600
C	1.18555400	3.54145800	-2.48348800
H	0.28128500	2.91264300	-2.49327000
H	1.52544500	3.65768300	-3.52410000
H	0.87999500	4.53732900	-2.12868200
C	4.02842500	-4.22297200	0.28908300
H	5.11583400	-4.27801900	0.34761500
C	-5.02281600	0.60827900	-0.72337100
H	-4.97876700	0.56821100	-1.82660000
C	4.02966500	1.06082500	0.68915600
H	3.48090500	0.19410200	0.28289700
H	4.76979100	0.68328800	1.41282800
H	4.58922700	1.50727300	-0.14732600
C	-3.51013700	0.68136200	2.53193100
H	-2.97320600	1.56013800	2.13841600
H	-3.19325500	0.53184700	3.57650000
H	-4.58153800	0.93168400	2.55308200
C	3.14330800	-0.87491500	-2.60741700
H	3.40051100	0.14951400	-2.30460100
H	3.43817600	-1.00824300	-3.65773400
H	3.73010100	-1.57762500	-2.00079800
C	-1.99448100	-2.68434200	-0.70480000
H	-1.94853900	-3.69041400	-1.15356400
H	-1.85940500	-2.79135200	0.38360900
H	-1.13571100	-2.11011300	-1.09245400
C	-3.46759400	-1.86601100	-2.58345700
H	-2.68625300	-1.22122900	-3.02021000
H	-4.44226900	-1.44401400	-2.86656800
H	-3.38427400	-2.85390700	-3.06232900
C	-4.05578000	-1.77410800	2.23590600
H	-5.14027200	-1.61282800	2.14405200
H	-3.84024300	-1.93110400	3.30499500
H	-3.81327000	-2.70908200	1.70870000
C	1.03178300	5.24445300	0.76583700
H	1.85896400	5.33155100	1.48515700
H	0.26008500	5.96956200	1.06679100
H	1.40884700	5.55785100	-0.21723300
C	-6.28234100	-0.14359300	-0.26894000
H	-6.27243600	-1.20437700	-0.56332000
H	-7.18356700	0.31171100	-0.70691700

H	-6.39565000	-0.09803000	0.82552900
C	1.32615000	-2.58101900	-2.87520400
H	1.98712500	-3.31182400	-2.39285200
H	1.47279900	-2.66539400	-3.96100000
H	0.28126500	-2.84131300	-2.65235600
C	-5.08422700	2.08503500	-0.31799900
H	-5.14764700	2.20396500	0.77317000
H	-5.97748200	2.56141600	-0.75015000
H	-4.20815800	2.65175600	-0.66831900