Electronic Supplementary Material (ESI) for Dalton Transactions.

Contents:

1. NMR spectra

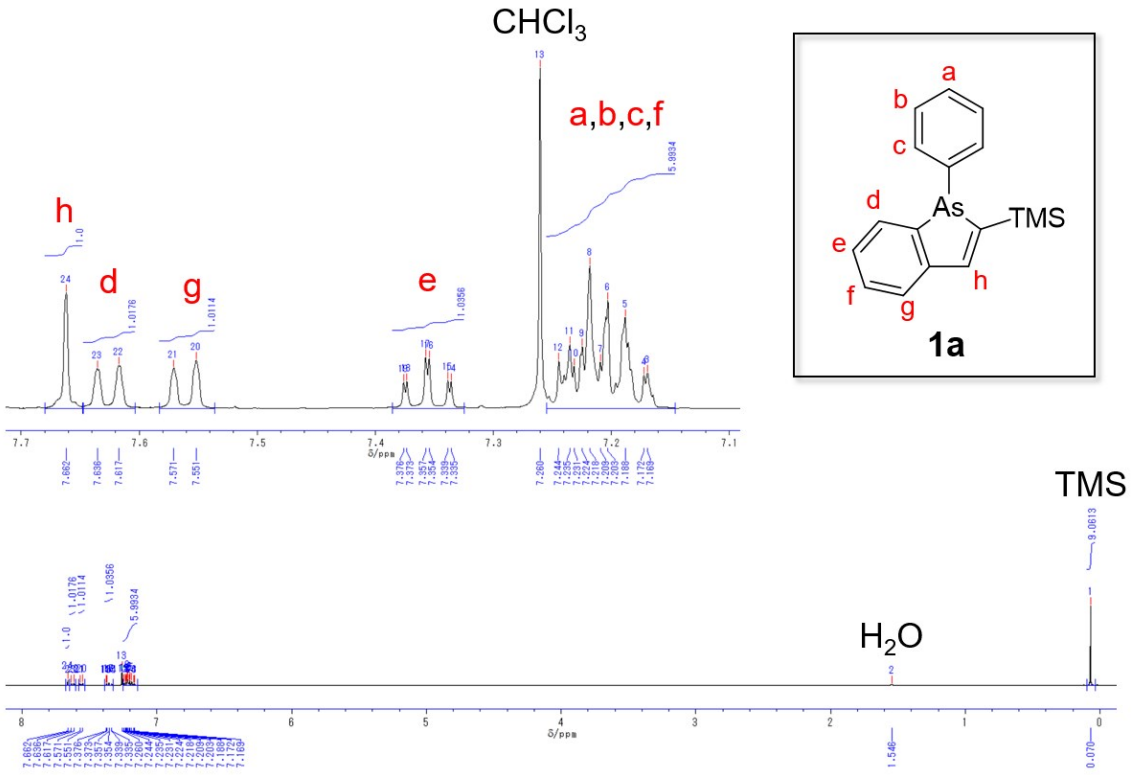


Figure S1. ^{1}H-NMR spectrum (400 MHz) of **1a** in $CDCl_3$.

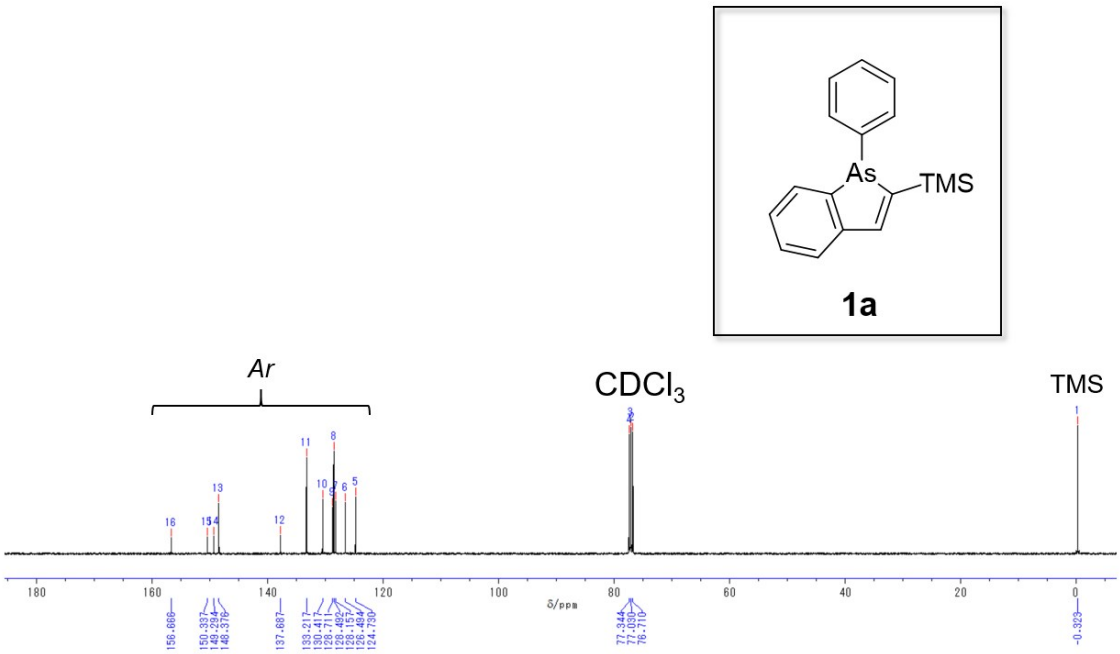


Figure S2. ^{13}C-NMR spectrum (100 MHz) of **1a** in $CDCl_3$.

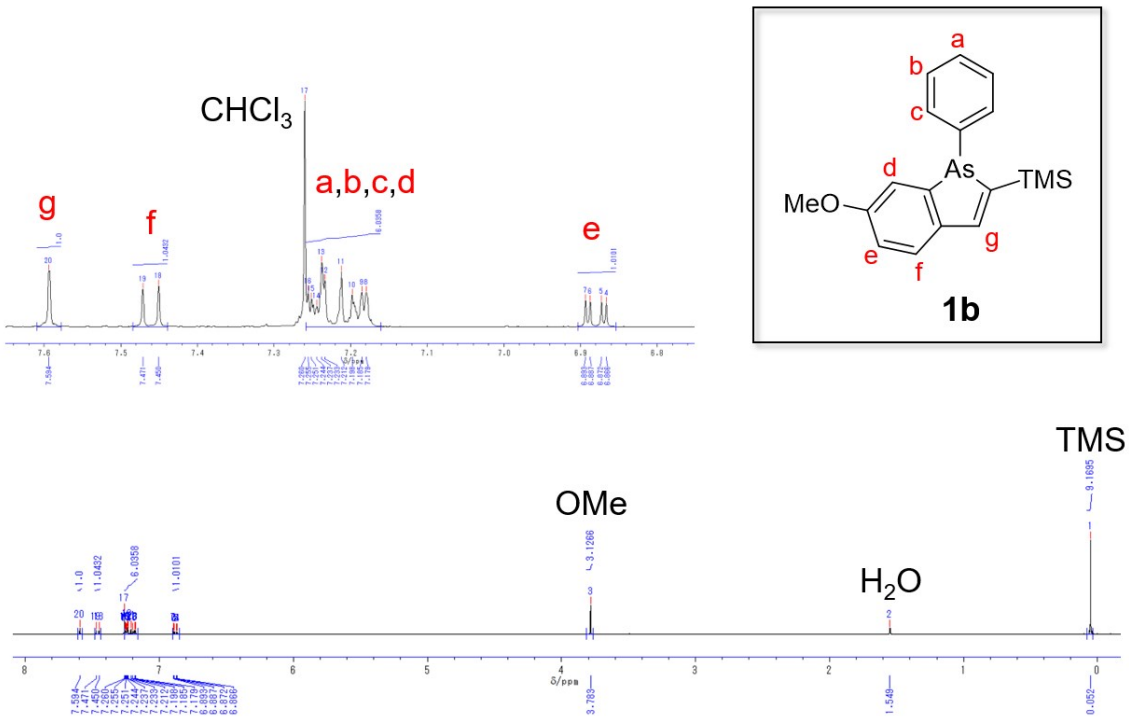


Figure S3. ^{1}H-NMR spectrum (400 MHz) of **1b** in $CDCl_3$.

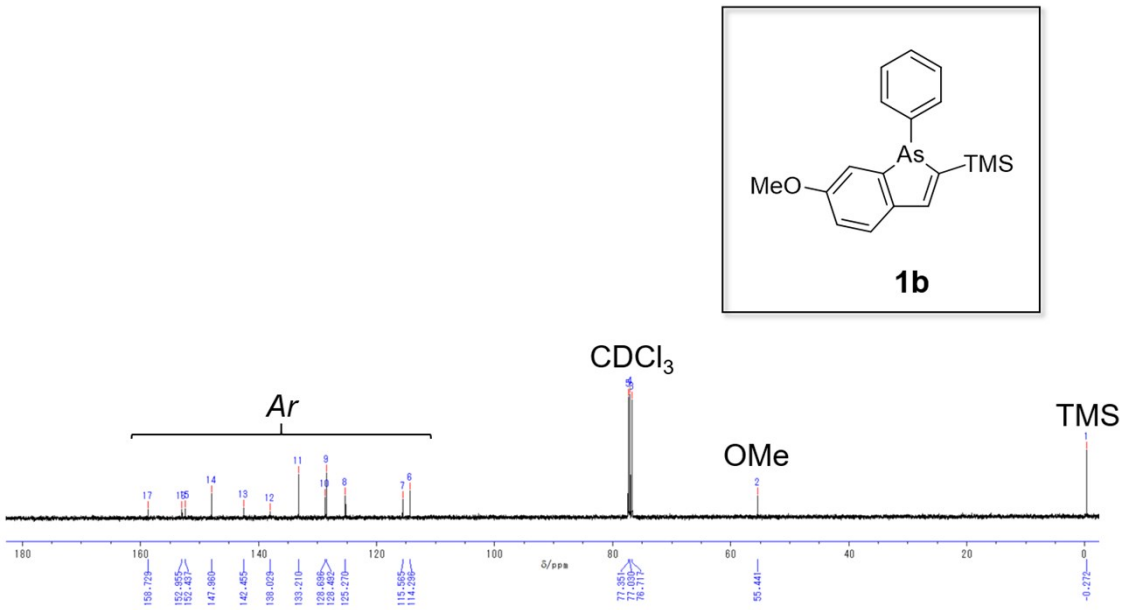


Figure S4. ^{13}C-NMR spectrum (100 MHz) of **1b** in $CDCl_3$.

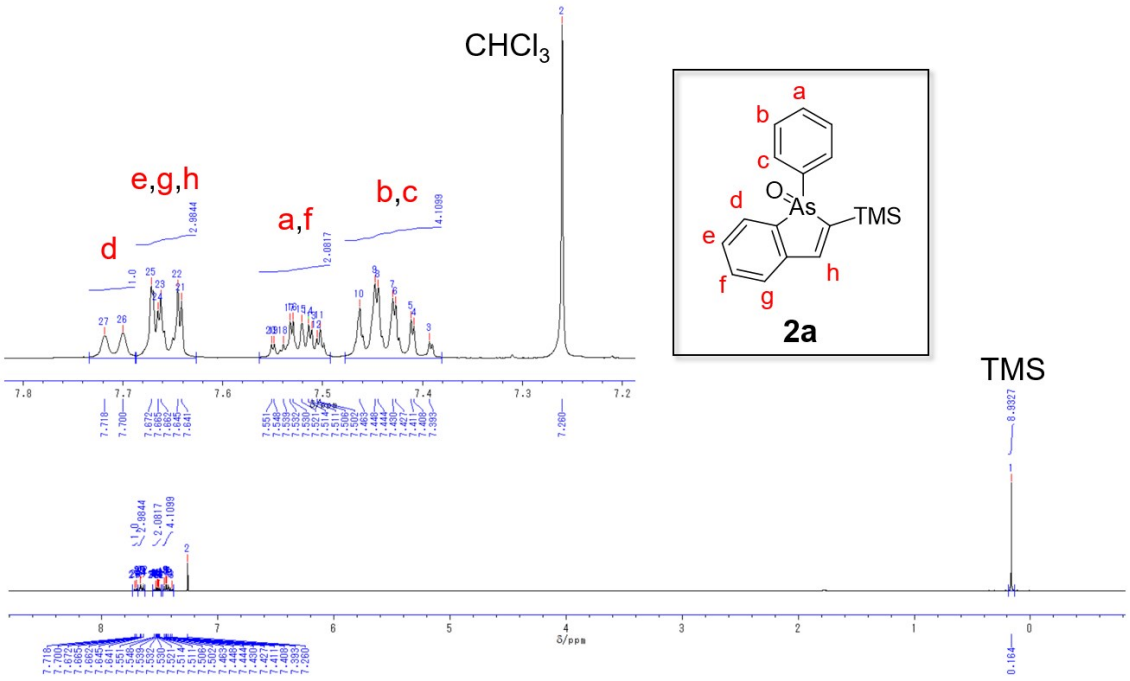


Figure S5. ^{1}H-NMR spectrum (400 MHz) of **2a** in $CDCl_3$.

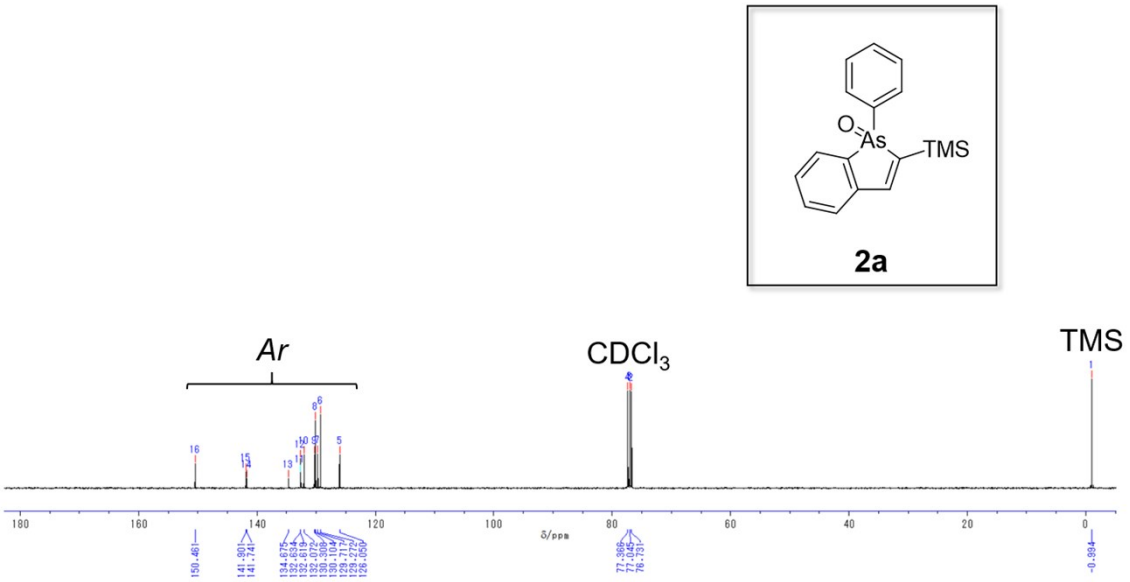


Figure S6. ^{13}C-NMR spectrum (100 MHz) of **2a** in $CDCl_3$.

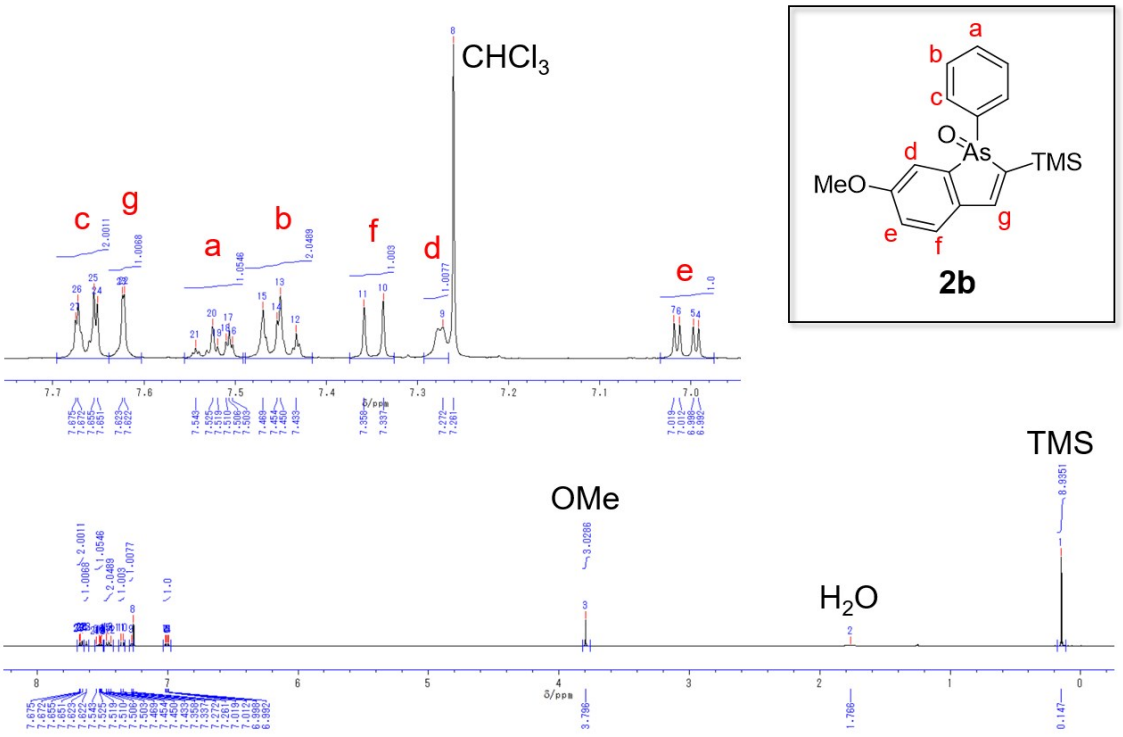


Figure S7. ^{1}H-NMR spectrum (400 MHz) of **2b** in $CDCl_3$.

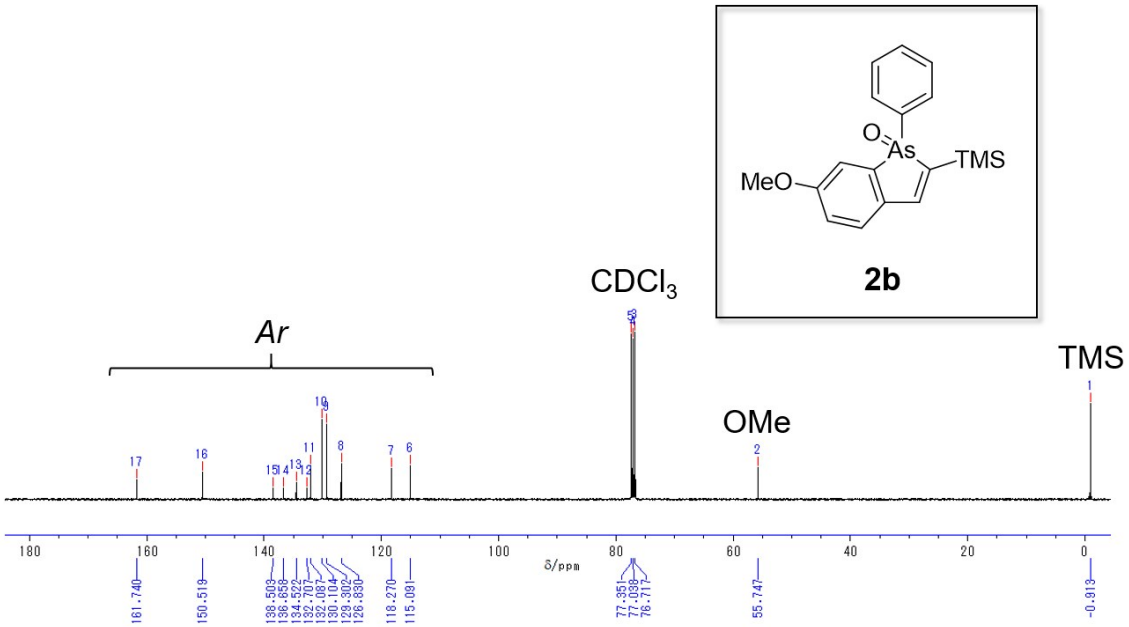


Figure S8. ^{13}C-NMR spectrum (100 MHz) of **2b** in $CDCl_3$.

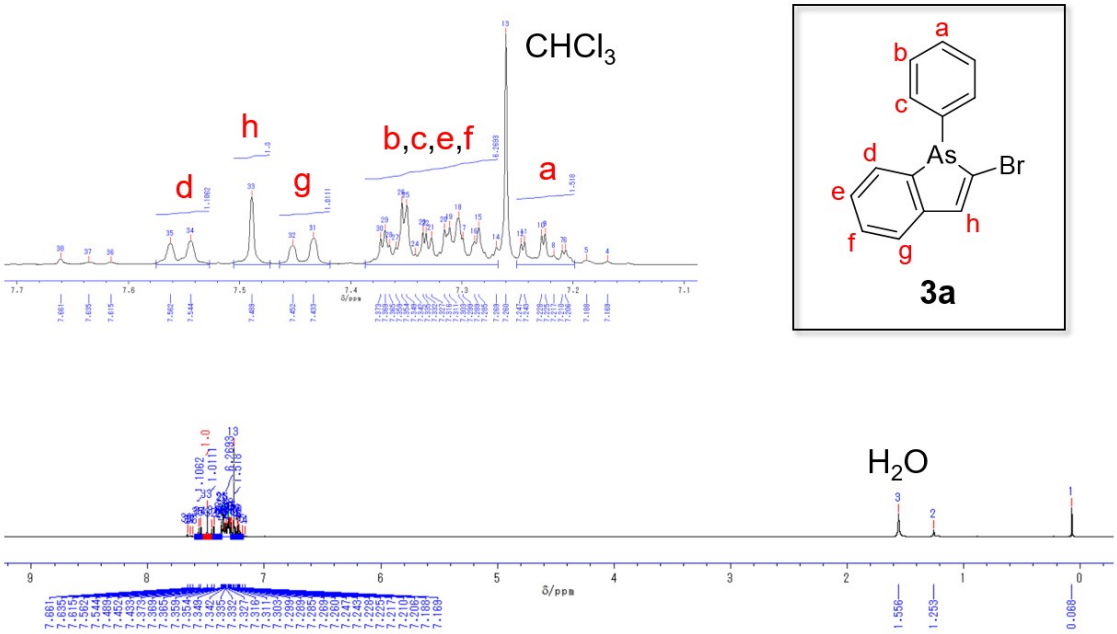


Figure S9. ^{1}H-NMR spectrum (400 MHz) of **3a** (crude) in $CDCl_3$.

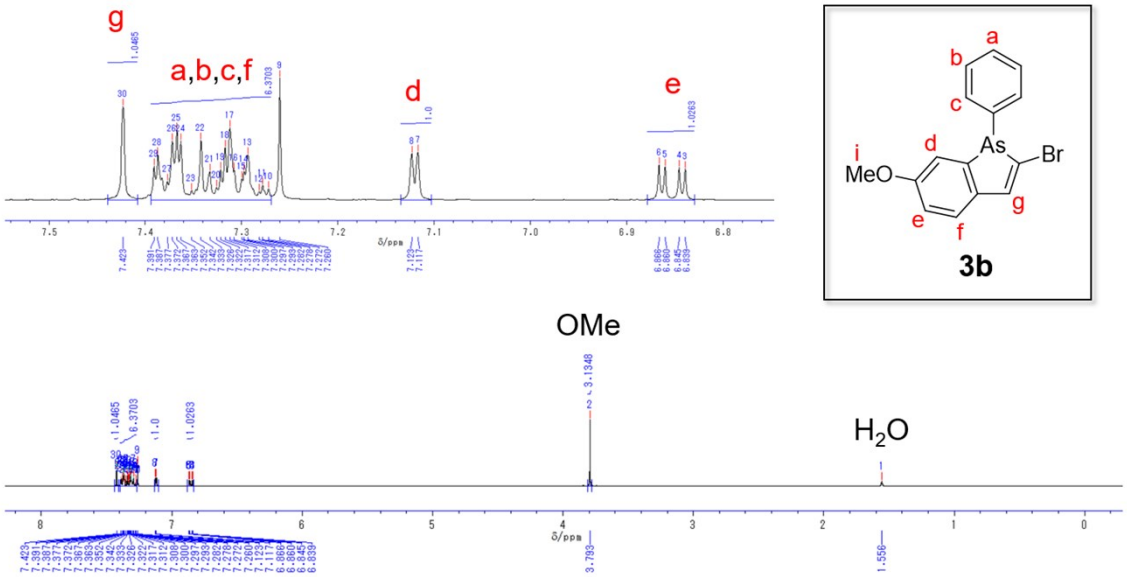


Figure S10. ^{1}H-NMR spectrum (400 MHz) of **3b** in $CDCl_3$.

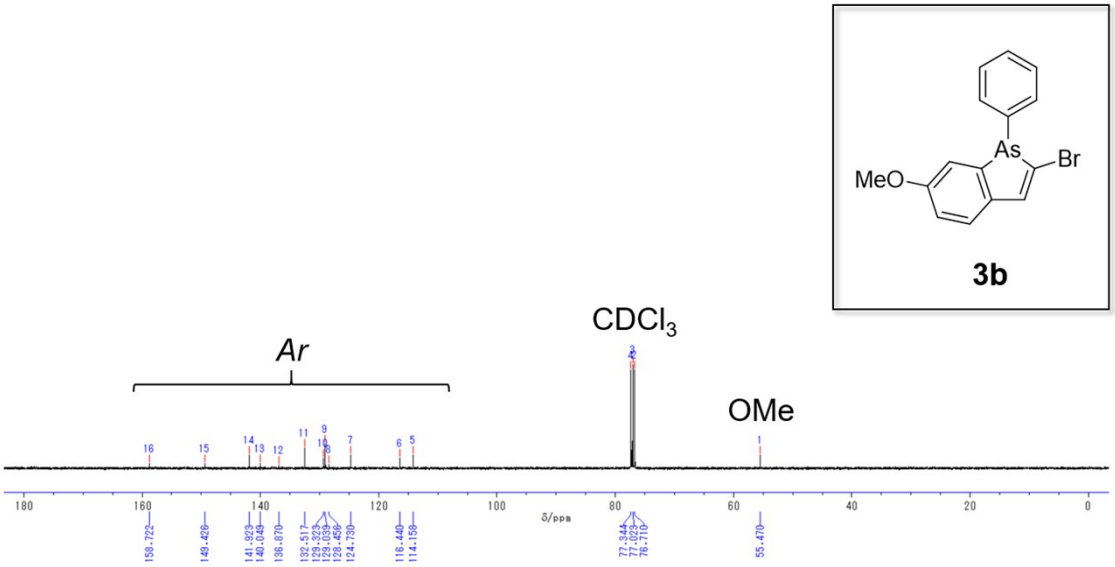


Figure S11. ^{13}C-NMR spectrum (100 MHz) of **3b** in $CDCl_3$.

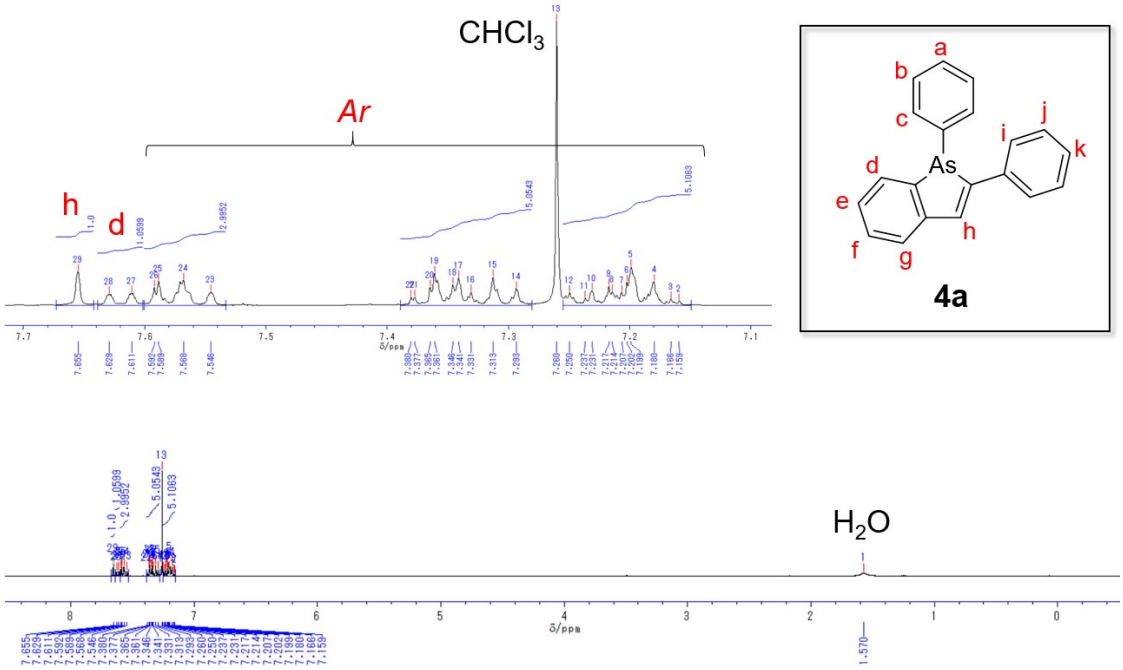


Figure S12. ^{1}H-NMR spectrum (400 MHz) of **4a** in $CDCl_3$.

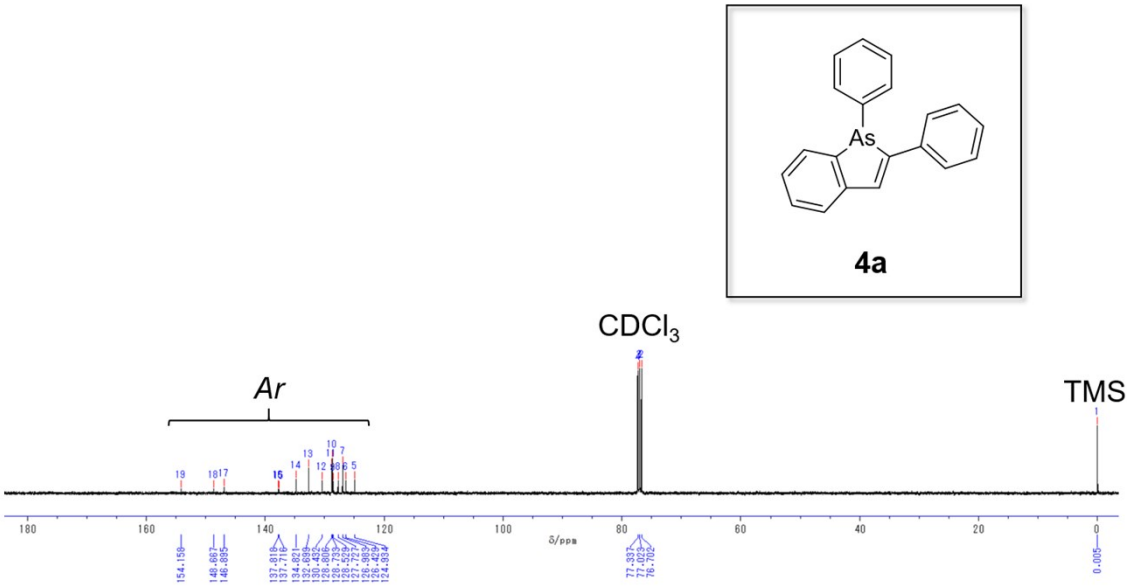


Figure S13. ^{13}C-NMR spectrum (100 MHz) of **4a** in $CDCl_3$.

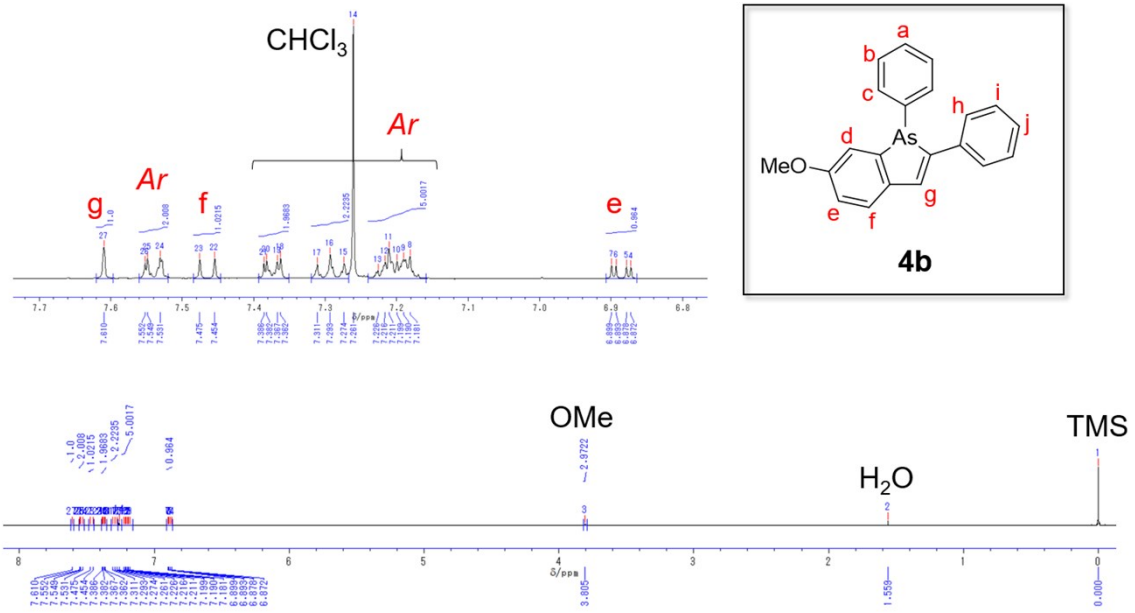


Figure S14. ^{1}H-NMR spectrum (400 MHz) of **4b** in $CDCl_3$.

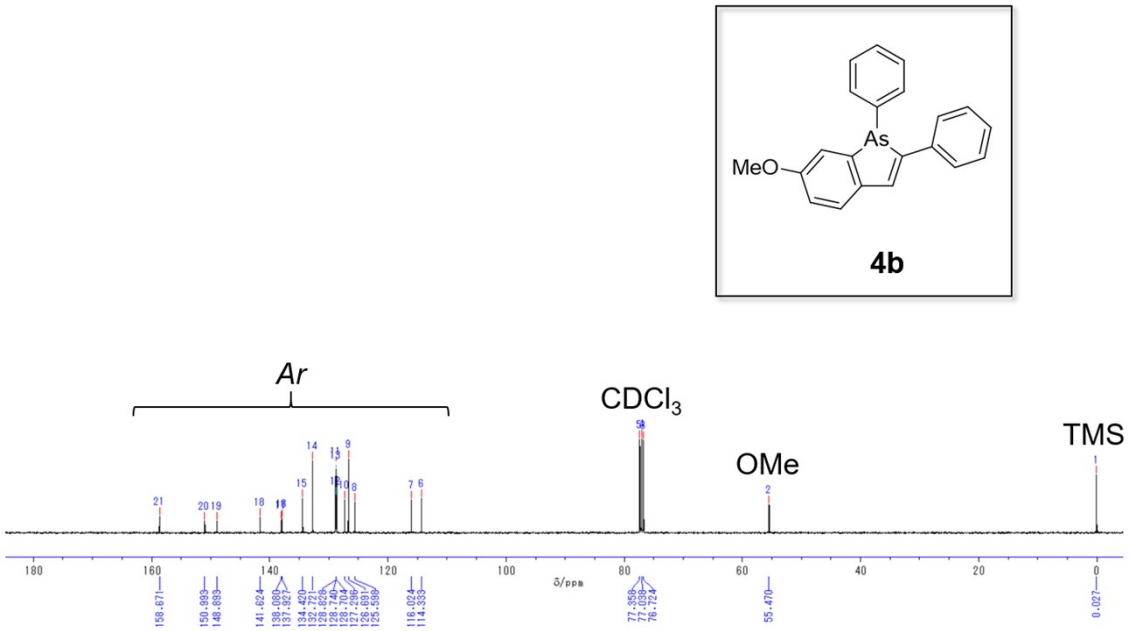


Figure S15. ^{13}C-NMR spectrum (100 MHz) of **4b** in $CDCl_3$.

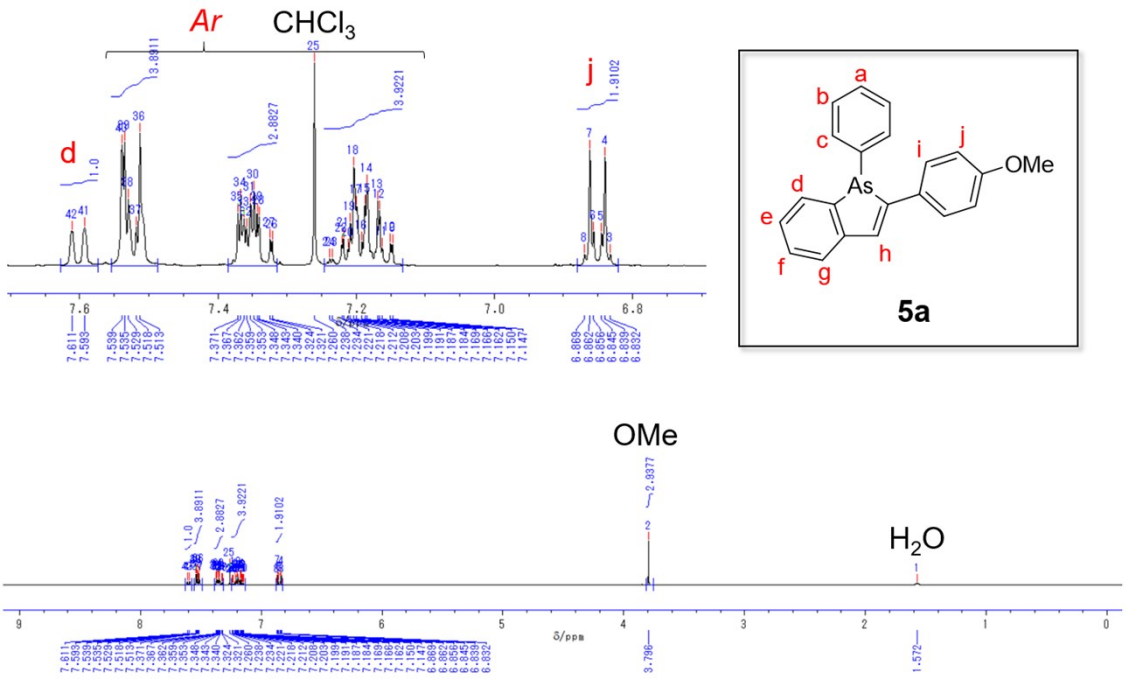


Figure S16. ^{1}H-NMR spectrum (400 MHz) of **5a** in $CDCl_3$.

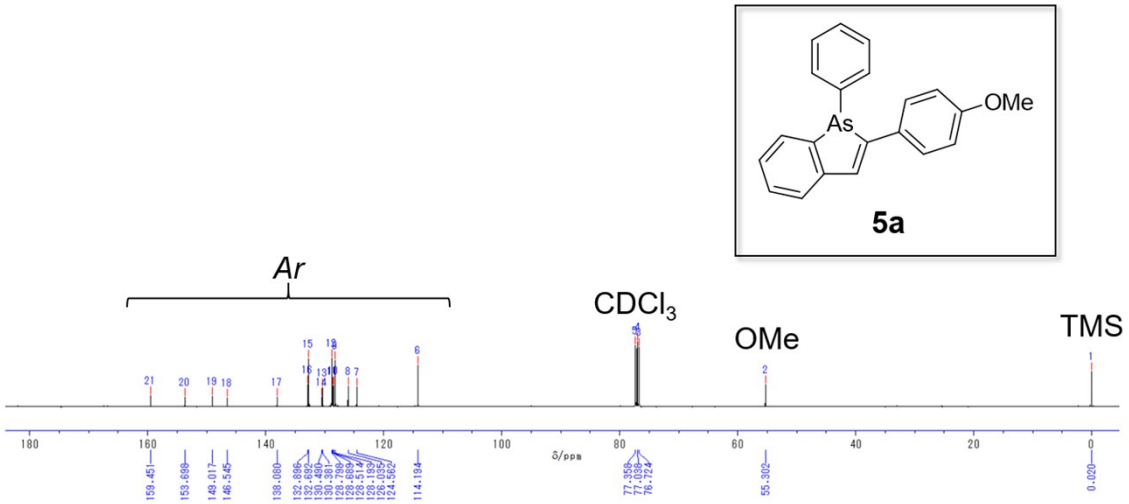


Figure S17. ^{13}C-NMR spectrum (100 MHz) of **5a** in $CDCl_3$.

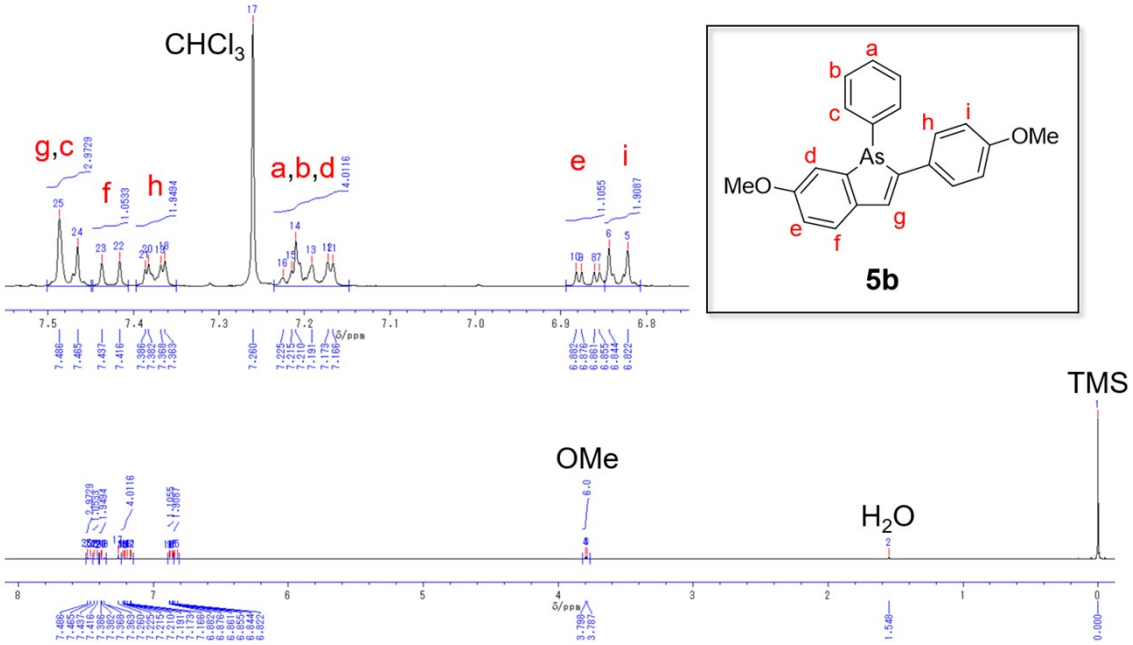


Figure S18. ^{1}H-NMR spectrum (400 MHz) of **5b** in $CDCl_3$.

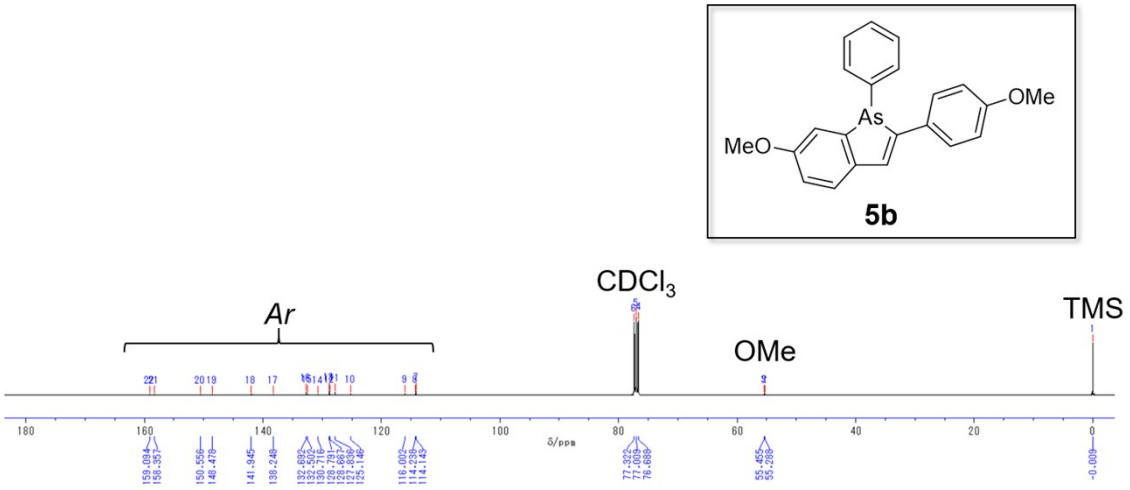


Figure S19. ^{13}C-NMR spectrum (100 MHz) of **5b** in $CDCl_3$.

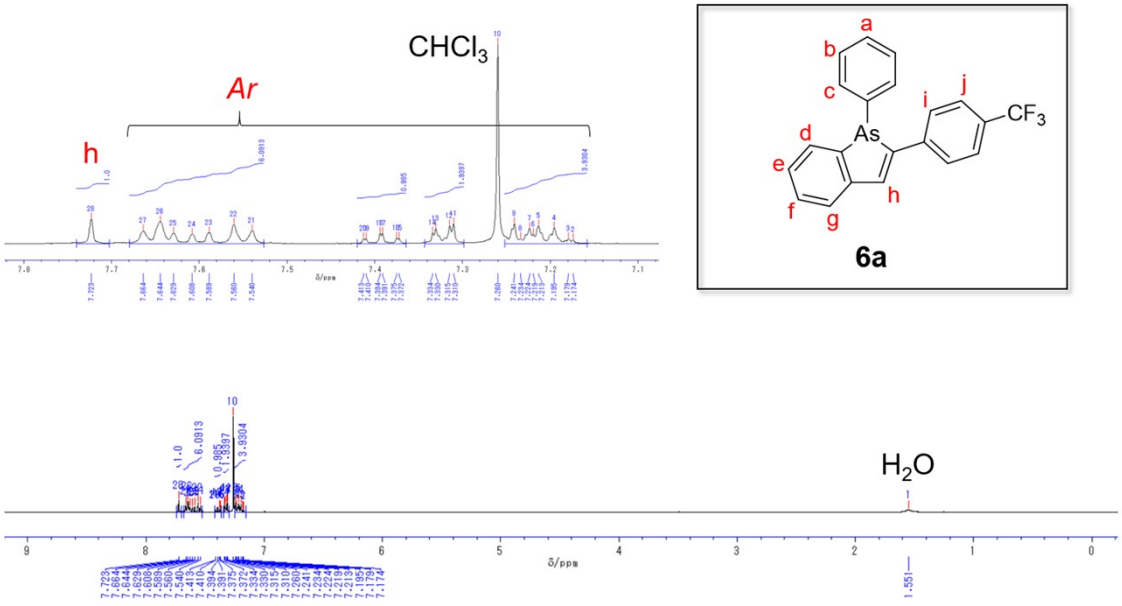


Figure S20. ^{1}H-NMR spectrum (400 MHz) of **6a** in $CDCl_3$.

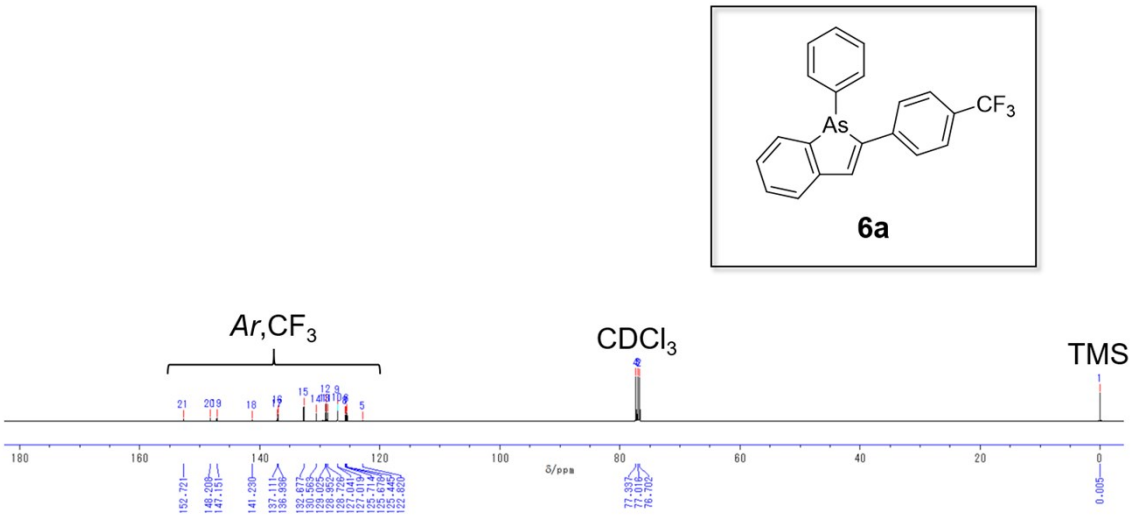


Figure S21. ^{13}C-NMR spectrum (100 MHz) of **6a** in $CDCl_3$.

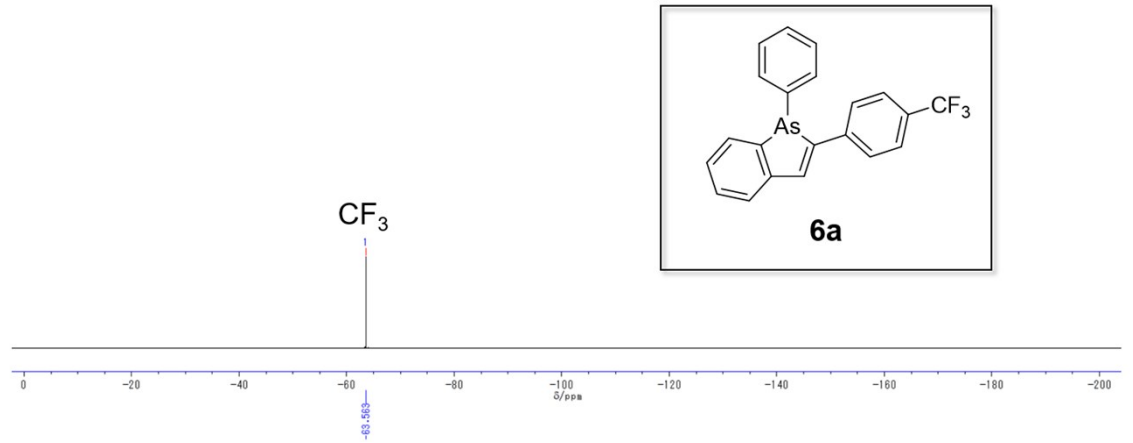


Figure S22. ^{19}F-NMR spectrum (376 MHz) of **6a** in $CDCl_3$.

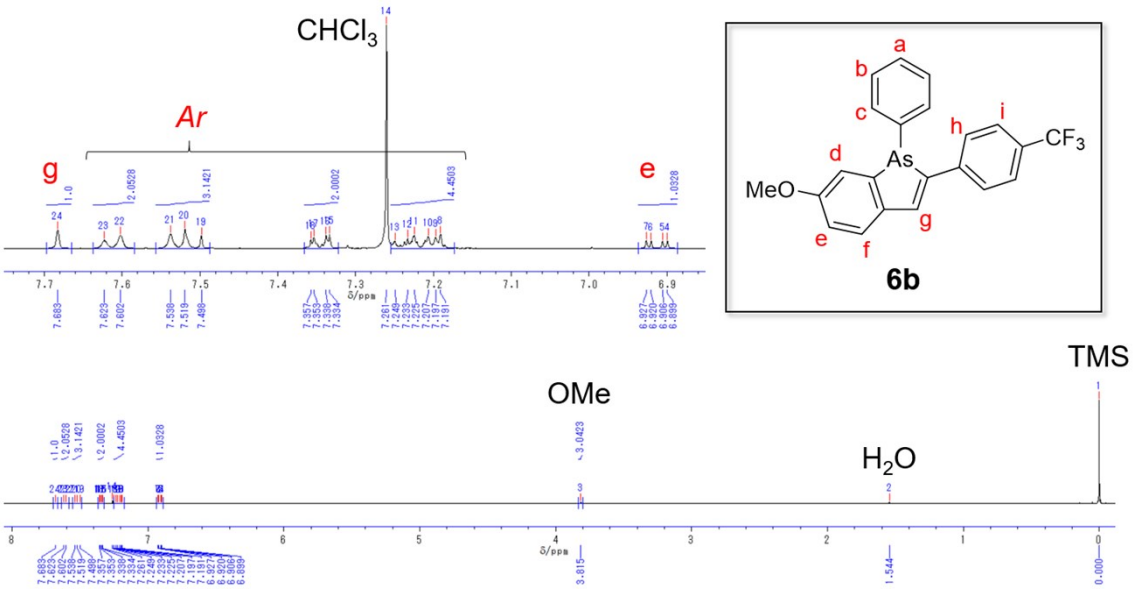


Figure S23. ^{1}H-NMR spectrum (400 MHz) of **6b** in $CDCl_3$.

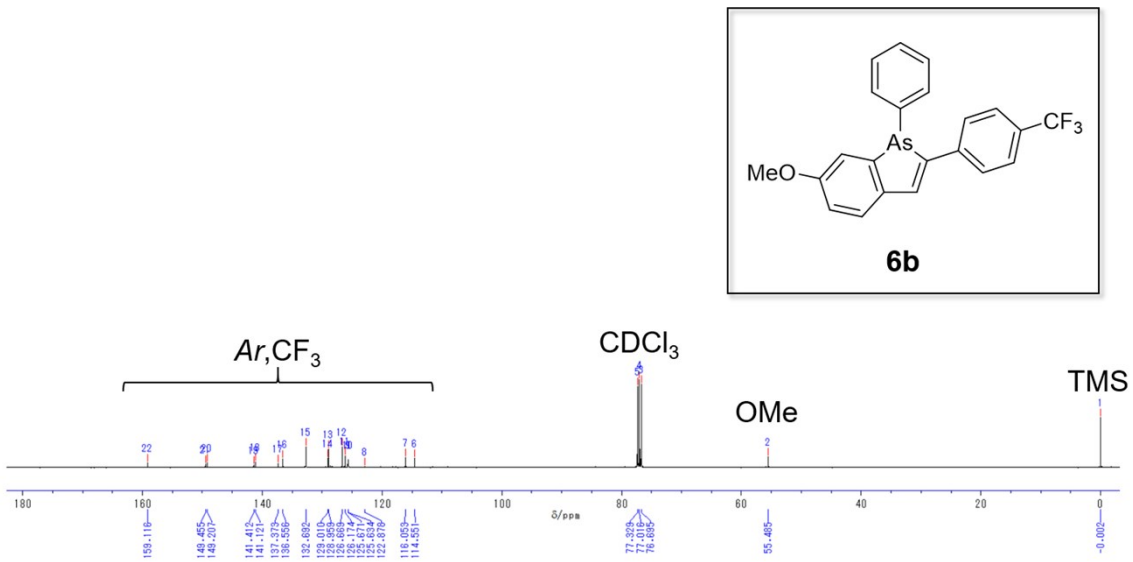


Figure S24. ^{13}C-NMR spectrum (100 MHz) of **6b** in $CDCl_3$.

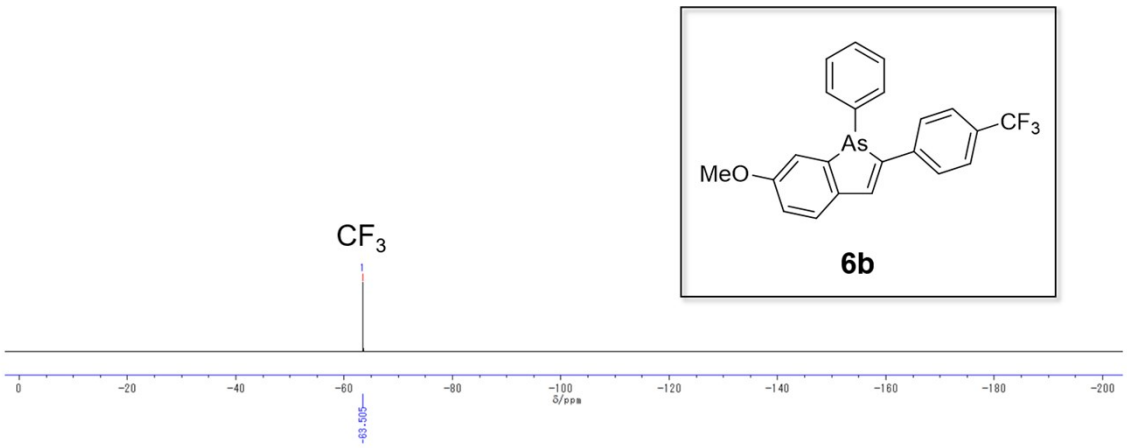


Figure S25. ^{19}F-NMR spectrum (376 MHz) of **6b** in $CDCl_3$.

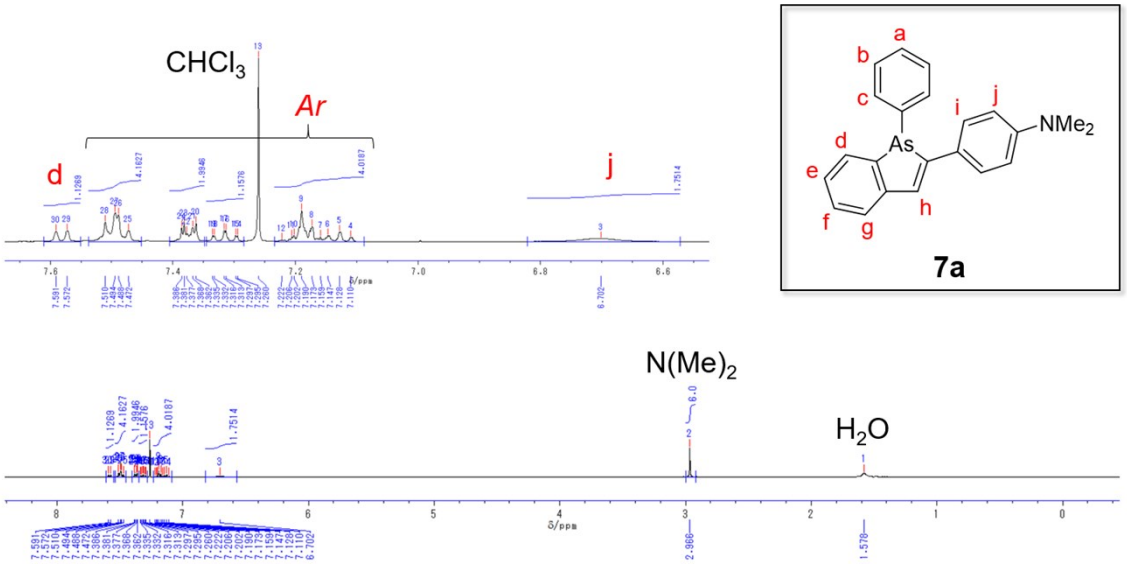


Figure S26. ^{1}H-NMR spectrum (400 MHz) of **7a** in $CDCl_3$.

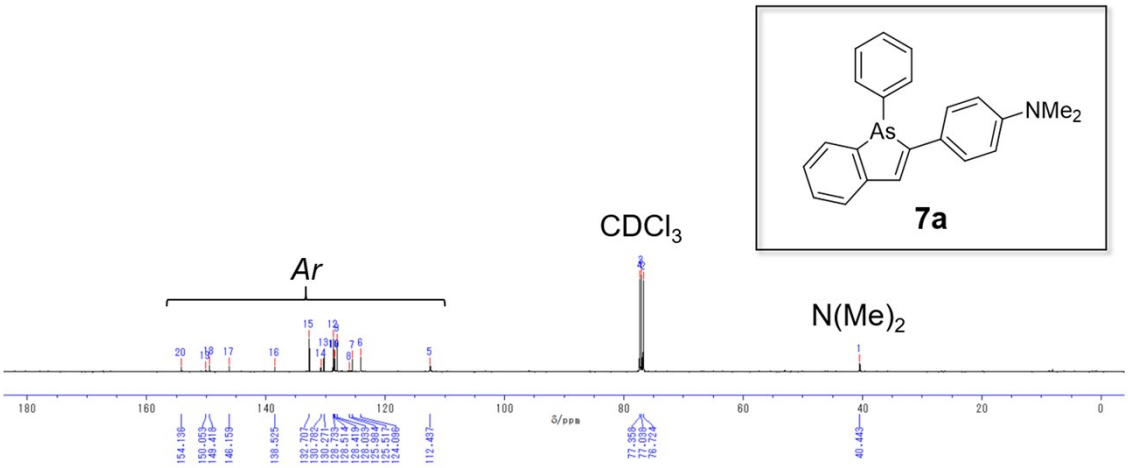


Figure S27. ^{13}C-NMR spectrum (100 MHz) of **7a** in $CDCl_3$.

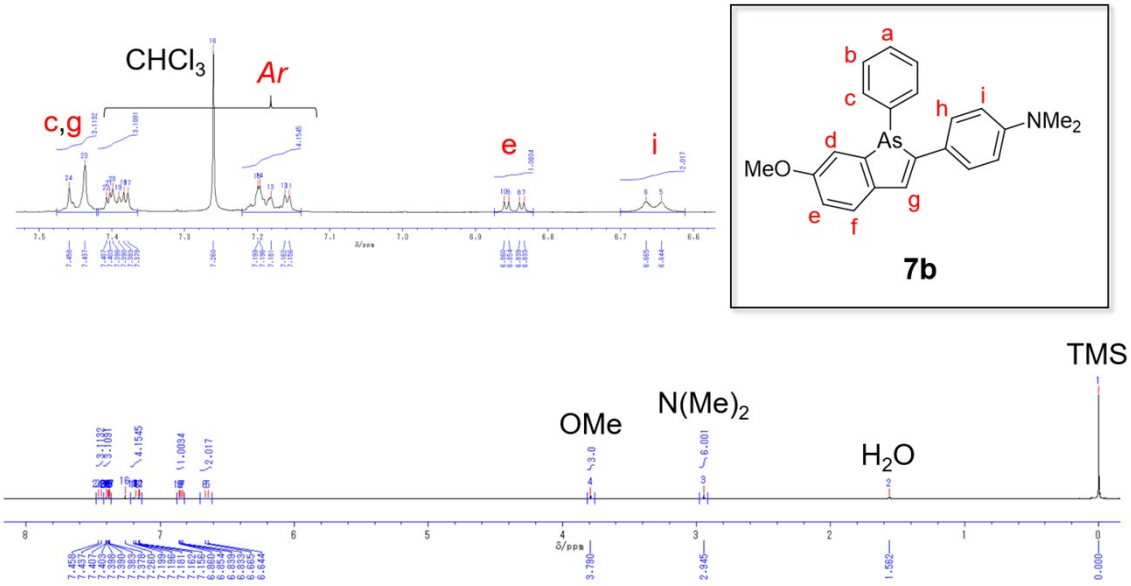


Figure S28. ^{1}H-NMR spectrum (400 MHz) of **7b** in $CDCl_3$.

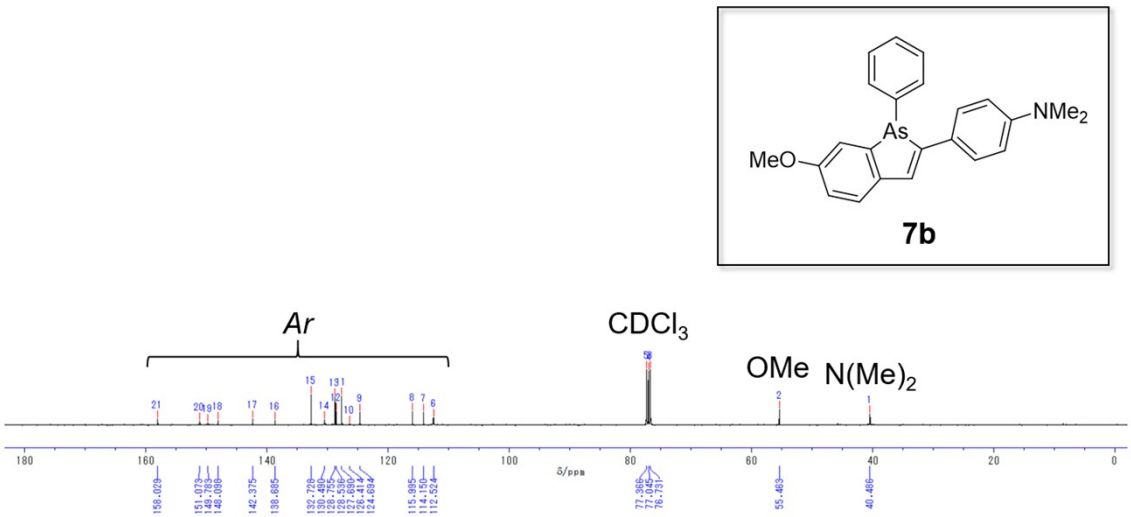


Figure S29. ^{13}C-NMR spectrum (100 MHz) of **7b** in $CDCl_3$.

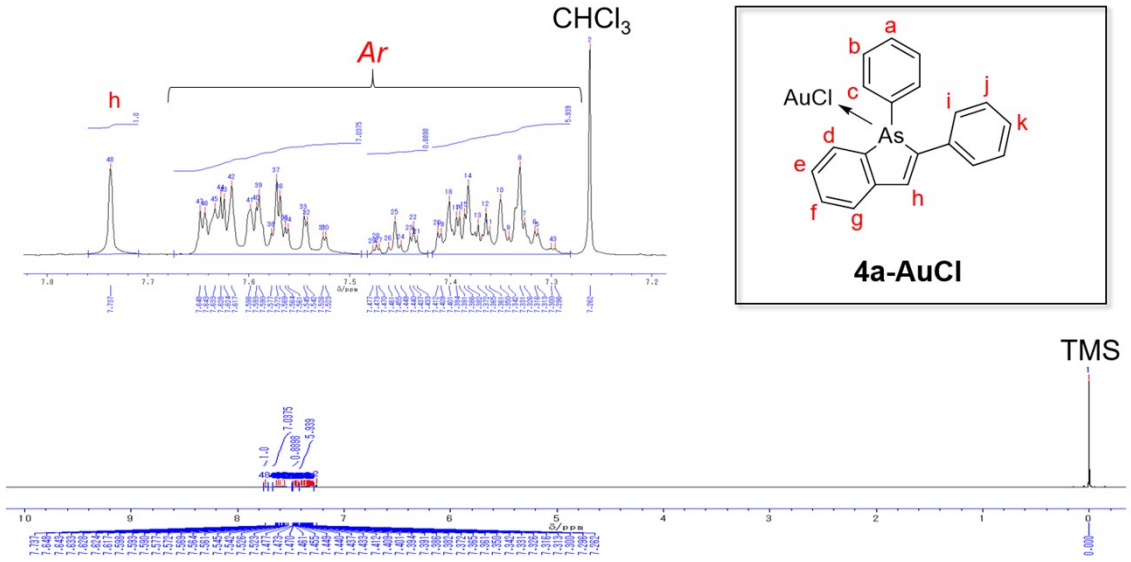


Figure S30. ^{1}H-NMR spectrum (400 MHz) of **4a-AuCl** in $CDCl_3$.

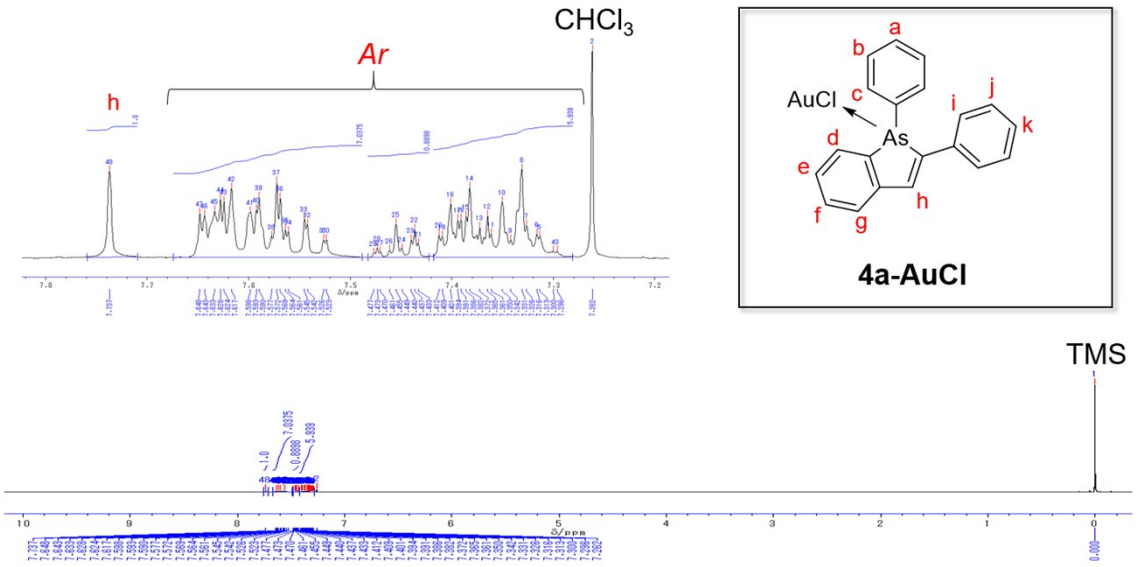


Figure S31. ^{13}C-NMR spectrum (100 MHz) of **4a-AuCl** in $CDCl_3$.

2. Crystallographic data

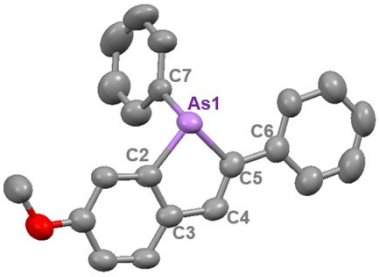
Table S1. Crystallographic Data of **4b**, **5a**, and **7a**.

Crystal data	**4b**	**5a**	**7a**
Empirical formula	$C_{21}H_{17}AsO$	$C_{21}H_{17}AsO$	$C_{22}H_{20}AsN$
Formula weight	360.29	360.29	373.33
Crystal Dimension, mm^3	0.360 × 0.120 × 0.110	0.280 × 0.210 × 0.170	0.250 × 0.190 × 0.050
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1$	$P2_1$
a, Å	15.323(4)	12.064(15)	10.302(3)
b, Å	6.0864(14)	6.135(7)	6.1145(14)
c, Å	18.537(5)	12.744(16)	14.508(3)
α, deg	-	-	-
β, deg	102.156(14)	114.742(12)	105.269(11)
γ, deg	-	-	-
Volume, $Å^3$	1690.0(8)	856.6(18)	881.6(4)
D_{calcd}, g cm^{-3}	1.416	1.397	1.406
Z	4	2	2
F(000)	736.00	368.00	384.00
Data collection			
Temperature, °C	25.0	25.0	25.0
$2\theta_{max}$, deg	55.2	55.0	55.0
T_{min}/T_{max}	0.801/0.661	0.713/0.621	0.908/0.769
Refinement			
No. of observed data	3777	3799	3909
No. of parameters	208	208	217
R1[a], wR2 [b]	0.0398, 0.0999	0.0314, 0.0680	0.0298, 0.0592
Goodness of fit indicator	1.064	1.015	0.973

[a]$R1 = \Sigma \mid |Fo| - |Fc| \mid / \Sigma|Fo|$, [b]$wR2 = [\Sigma w ((Fo^2 - Fc^2)^2 / \Sigma w (Fo^2)^2]^{1/2}$, $w = [\delta^2(Fo^2)]^{-1}$

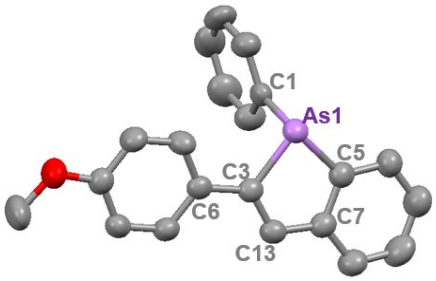
CCDC # 2005446 (**4b**), 2005444 (**5a**), 2005445 (**7a**)

Table S2. ORTEP drawing (ellipsoids at 50% probability), selected distances, and angles of **4b**.



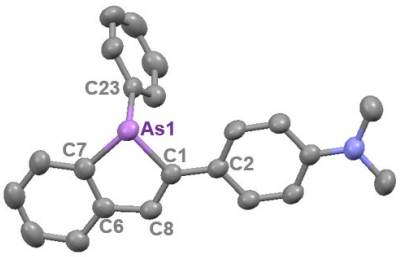
distances (Å)		angles (°)	
As1–C2	1.938(3)	C2–As1–C5	86.2(1)
As1–C5	1.954(3)	C2–As1–C7	99.4(1)
As1–C7	1.956(3)	C5–As1–C7	101.4(1)
C2–C3	1.394(4)	As1–C2–C3	110.6(2)
C3–C4	1.435(4)	C2–C3–C4	115.0(2)
C4–C5	1.354(4)	C3–C4–C5	117.9(3)
C5–C6	1.463(5)	As1–C5–C4	110.0(2)
		As1–C5–C6	122.1(2)
		C4–C5–C6	127.6(3)

Table S3. ORTEP drawing (ellipsoids at 50% probability), selected distances, and angles of **5a**.



distances (Å)		angles (°)	
As1–C5	1.948(5)	C3–As1–C5	86.0(2)
As1–C3	1.956(4)	C1–As1–C3	97.6(2)
As1–C1	1.969(6)	C1–As1–C5	101.6(2)
C5–C7	1.402(6)	As1–C5–C7	110.6(3)
C7–C13	1.457(5)	C5–C7–C13	114.7(4)
C13–C3	1.348(6)	C7–C13–C3	117.3(4)
C3–C6	1.484(5)	As1–C3–C13	111.0(3)
		As1–C3–C6	122.1(3)
		C6–C3–C13	126.9(3)

Table S4. ORTEP drawing (ellipsoids at 50% probability), selected distances, and angles of **7a**.



distances (Å)		angles (°)	
As1–C7	1.955(4)	C7–As1–C1	86.6(2)
As1–C1	1.959(3)	C7–As1–C23	98.5(2)
As1–C23	1.962(5)	C1–As1–C23	101.6(2)
C6–C7	1.401(6)	As1–C7–C6	110.1(3)
C6–C8	1.460(5)	C7–C6–C8	114.8(4)
C1–C8	1.350(5)	C1–C8–C6	118.1(4)
C1–C2	1.462(4)	As1–C1–C8	109.9(3)
		As1–C1–C2	122.5(2)
		C2–C1–C8	127.5(3)

3. Photophysical data

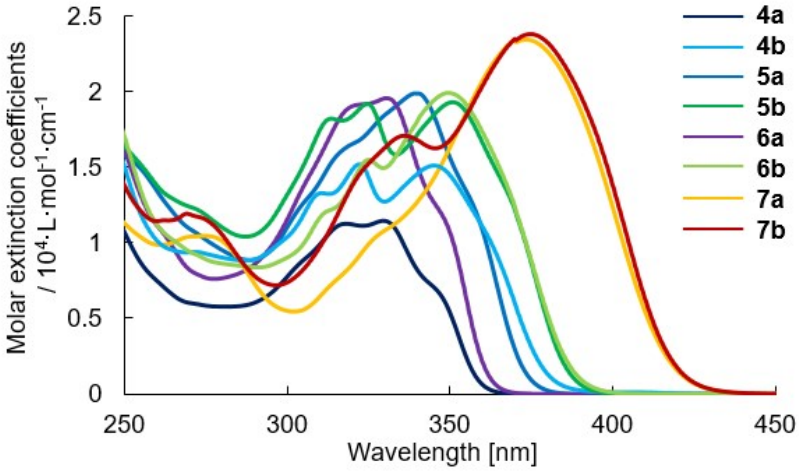


Figure S32. UV-vis absorption spectra of **4-7** in CH_2Cl_2 solutions (c = 1.0 × 10^{-5} M).

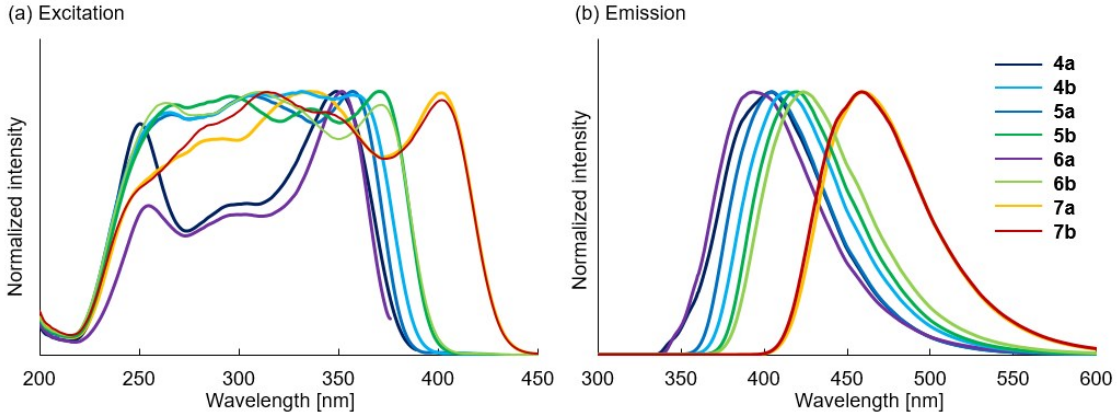


Figure S33. (a) Excitation (monitored at emission maxima) and (b) emission spectra (excited at excitation maxima) of **4-7** at room temperature in CH_2Cl_2 solutions (c = 1.0 × 10^{-4} M).

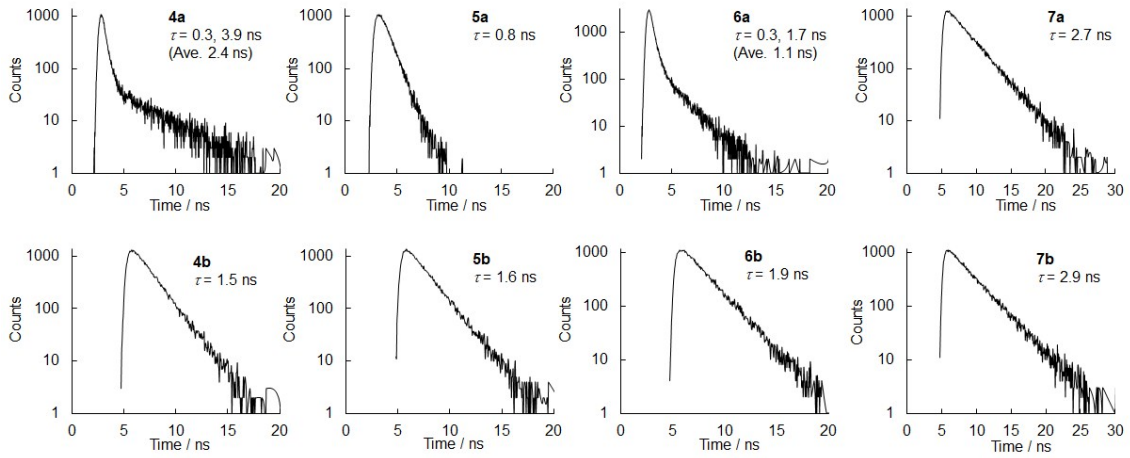


Figure S34. The emission decay kinetics of **4**-**7** at room temperature (exited at 340 nm, monitored at λ_{em}) in CH_2Cl_2 solutions (c = 1.0 × 10^{-4} M).

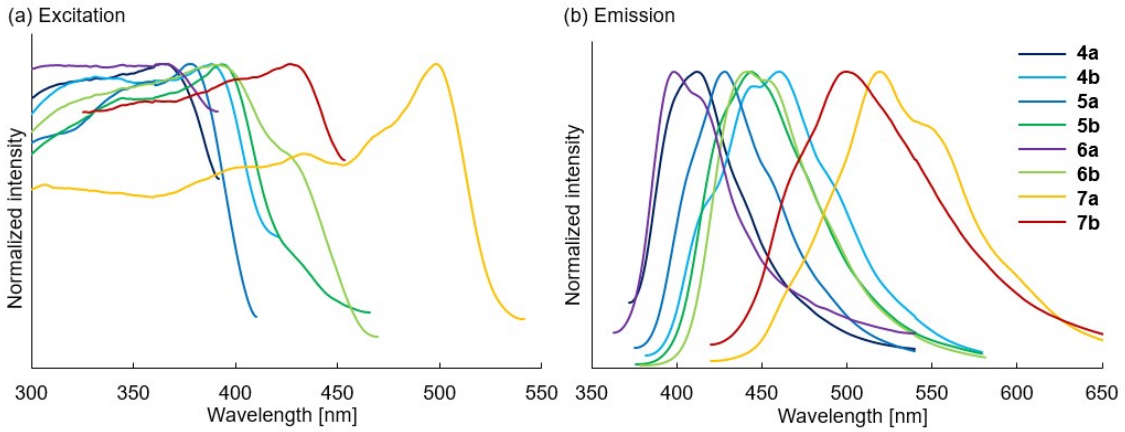


Figure S35. (a) Excitation (monitored at emission maxima) and (b) emission spectra (excited at excitation maxima) of **4**-**7** at room temperature in the solid states.

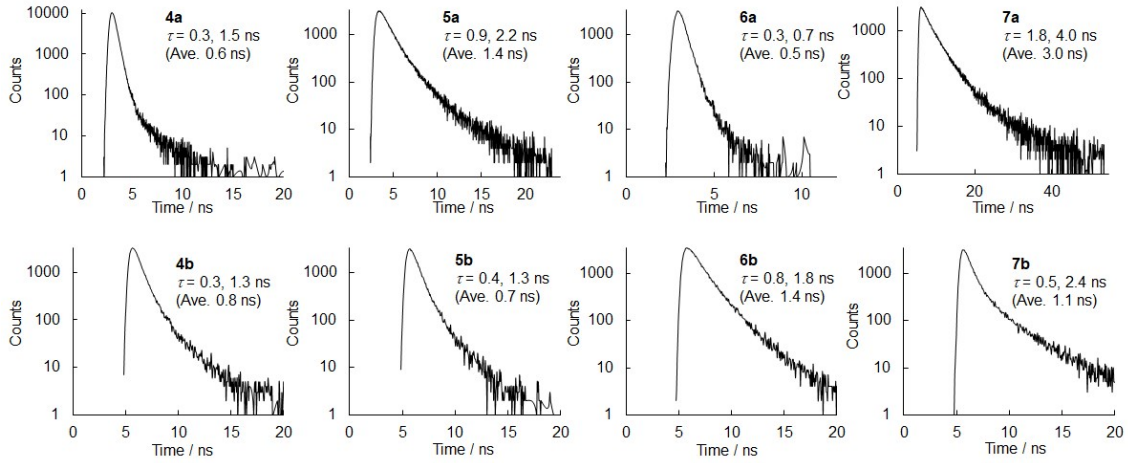


Figure S36. The emission decay kinetics of **4-7** at room temperature (exited at 340 nm, monitored at λ_{em}) in the solid states.

Table S5. PL properties of **4-7** at room temperature in the solid states.

	λ_{ex} [nm]	λ_{em} [nm]	Φ	τ [ns]
4a	366	409	0.03	0.6
5a	379	426	0.13	1.4
6a	366	399	< 0.01	0.5
7a	498	519	0.13	3.0
4b	390	461	0.18	0.8
5b	393	444	0.14	0.7
6b	389	453	0.16	1.4
7b	427	500	0.03	1.1

Table S6. Radiative (k_r) and non-radiative (k_{nr}) rate constants of **4-7** at room temperature in solutions and solid states.

	Solution		Solid	
	k_r [10^8/sec]	k_{nr} [10^8/sec]	k_r [10^8/sec]	k_{nr} [10^8/sec]
4a	n.d.	n.d.	1.5	16.2
5a	3.0	9.5	0.9	6.2
6a	n.d.	n.d.	n.d.	n.d.
7a	3.3	0.4	0.4	2.9
4b	2.7	3.9	2.3	10.3
5b	2.5	3.8	2.0	12.3
6b	3.3	1.9	1.1	6.0
7b	2.8	0.6	0.3	8.8

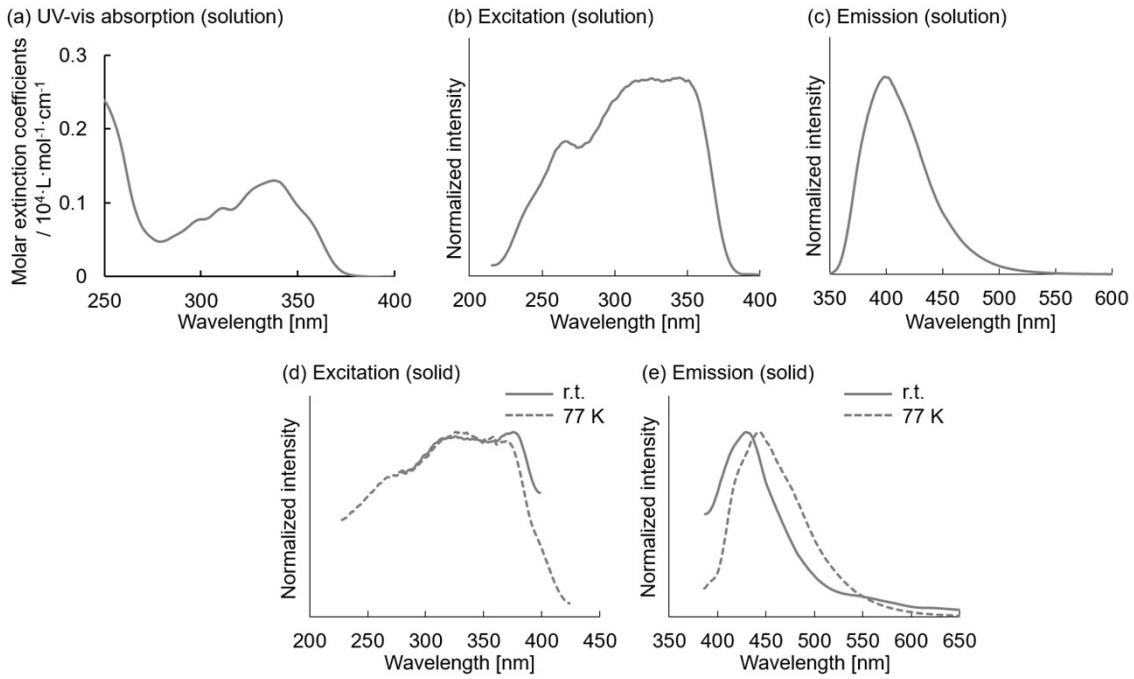


Figure S37. Spectra of **4a-AuCl** in a CH_2Cl_2 solution (a-c) and the solid state (d, e): (a) UV-vis absorption (c = 1.0 × 10^{-5} M), (b) excitation (c = 1.0 × 10^{-4} M, monitored at emission maximum), (c) emission (c = 1.0 × 10^{-4} M, excited at excitation maximum), (d) excitation (monitored at emission maximum), and (e) emission (excited at excitation maximum) spectra.

4. DFT calculations

Table S7. Results of DFT and TD-DFT calculations.[a]

	HOMO [eV]	LUMO [eV]	*E* [nm][b]	*f*[c]
4a	-5.83322	-1.7211	334.81	0.3962
5a	-5.52084	-1.57933	349.46	0.4704
6a	-6.16356	-2.12518	339.63	0.4622
7a	-5.06778	-1.42123	376.65	0.5687
4b	-5.5056	-1.55865	352.86	0.3858
5b	-5.27322	-1.42967	362.59	0.4424
6b	-5.78125	-1.99429	364.98	0.4852
7b	-4.90914	-1.28545	383.29	0.5389

[a]The full geometries were optimized by DFT calculation, and all the calculations were performed at the B3LYP/6-31G+(d,p) level of theory. [b]Electron transition energy due to HOMO-LUMO transition. [c]Oscillator strength of HOMO-LUMO transition.

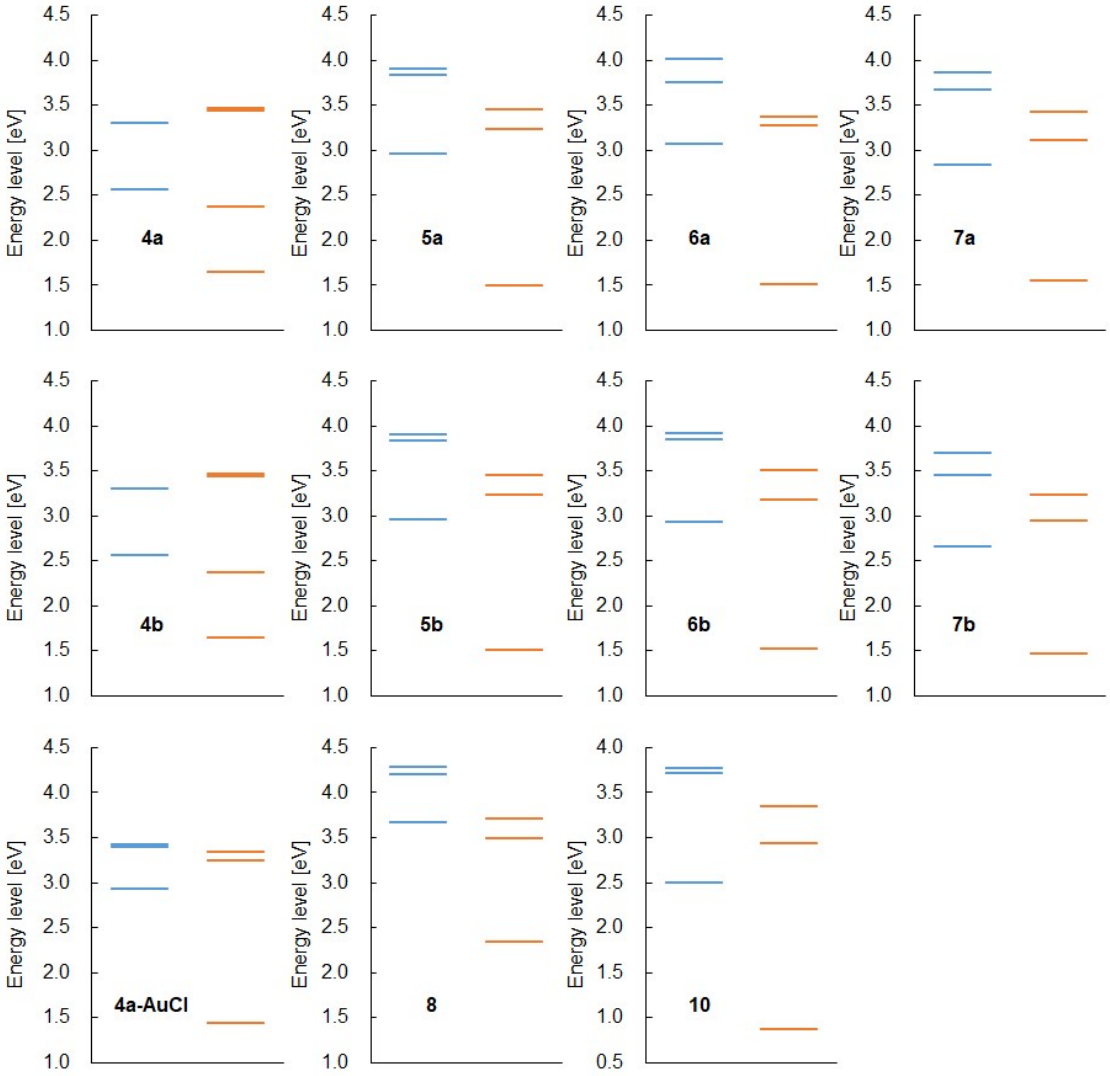


Figure S38. Energy levels of **4-7**, **4a-AuCl**, **8**, and **10** in the singlet (blue line) and triplet (red line) excitation states against the ground states. The full geometries were optimized at the S_1 states.

In the case of **6a**, the energy level of the T_2 state was higher than that of the S_1 one though its quantum yield was low (< 0.01). It is possible that the intersystem crossing can occur from S_1 to T_2 at room temperature because the energy gap between the S_1 and T_2 states was relatively small (0.20 eV) when compared with highly emissive compounds (> 0.27 eV).

Cartesian coordinates in the structures optimized by DFT calculations

4a (S_0): *E*(B3LYP) = -3005.021379 hartree

Number	Atom	X	Y	Z
1	C	2.004064	-0.72826	-0.43995
2	C	1.655013	-1.80964	0.402163
3	C	0.21832	-1.99224	0.589408
4	C	-0.60971	-1.1128	-0.02995
5	As	0.411764	0.108959	-1.18154
6	C	0.3278	1.764679	-0.12663
7	C	0.133552	2.965919	-0.8184
8	C	0.061143	4.181355	-0.12872
9	C	0.184816	4.201376	1.261652
10	C	0.380345	3.004141	1.959886
11	C	0.45197	1.794558	1.26783
12	C	3.339063	-0.4342	-0.69427
13	C	4.344562	-1.21821	-0.11355
14	C	4.006057	-2.2942	0.715372
15	C	2.666399	-2.60154	0.965707
16	C	-2.07413	-1.09703	0.037523
17	C	-2.84265	-0.58867	-1.02866
18	C	-4.23648	-0.60903	-0.98424
19	C	-4.89967	-1.12035	0.13433
20	C	-4.15218	-1.61636	1.2076
21	C	-2.75939	-1.59103	1.16628
22	H	-0.15095	-2.82044	1.192008
23	H	0.033093	2.955872	-1.90075
24	H	-0.09158	5.106542	-0.67741
25	H	0.127652	5.1429	1.800482
26	H	0.47656	3.014685	3.042118
27	H	0.603088	0.870059	1.817692
28	H	3.610184	0.393503	-1.34443
29	H	5.388865	-0.98724	-0.30305
30	H	4.789661	-2.90192	1.158782
31	H	2.408285	-3.44412	1.602383

32	H	-2.33734	-0.2056	-1.91061
33	H	-4.80562	-0.22132	-1.82444
34	H	-5.98502	-1.1331	0.169977
35	H	-4.65608	-2.00591	2.087798
36	H	-2.19239	-1.95031	2.01991

4b (S_0): *E*(B3LYP) = -3119.551014 hartree

Number	Atom	X	Y	Z
1	C	1.5272	-0.6438	-0.2694
2	C	1.1671	-1.7291	0.555
3	C	-0.2694	-1.9618	0.6643
4	C	-1.093	-1.1208	-0.0119
5	As	-0.0516	0.1327	-1.1057
6	C	2.8619	-0.3017	-0.4752
7	C	3.8633	-1.05	0.1622
8	C	3.5165	-2.133	0.9891
9	C	2.1826	-2.4741	1.1792
10	C	-0.2467	1.7883	-0.0645
11	C	-0.4388	2.9796	-0.7739
12	C	-0.5933	4.1946	-0.0972
13	C	-0.5532	4.2242	1.2978
14	C	-0.3579	3.0374	2.0137
15	C	-0.2053	1.828	1.3346
16	O	5.2034	-0.8088	0.0375
17	C	-2.5581	-1.1553	-0.0317
18	C	-3.2772	-0.7279	-1.166
19	C	-4.6694	-0.7996	-1.2038
20	C	-5.3816	-1.2809	-0.102
21	C	-4.6846	-1.694	1.038
22	C	-3.2936	-1.6148	1.0794
23	C	5.6287	0.2575	-0.8024
24	H	-0.6443	-2.8	1.2497
25	H	3.1177	0.5294	-1.1225
26	H	4.3141	-2.6958	1.4631

27	H	1.9292	-3.3193	1.8141
28	H	-0.4751	2.9608	-1.8601
29	H	-0.7444	5.1121	-0.6592
30	H	-0.6742	5.1656	1.8265
31	H	-0.3264	3.0557	3.0997
32	H	-0.0595	0.9105	1.8975
33	H	-2.7309	-0.3679	-2.0333
34	H	-5.1999	-0.4739	-2.0942
35	H	-6.4659	-1.3347	-0.1316
36	H	-5.2277	-2.0588	1.9055
37	H	-2.7661	-1.9078	1.9824
38	H	6.7181	0.2594	-0.7512
39	H	5.3134	0.0977	-1.8412
40	H	5.2457	1.2229	-0.4484

5a (S_0): *E*(B3LYP) = -3119.550656 hartree

Number	Atom	X	Y	Z
1	C	2.4979	-0.963	-0.4043
2	C	1.9615	-1.9885	0.4087
3	C	0.5067	-1.9679	0.5296
4	C	-0.1615	-0.9717	-0.1073
5	As	1.0754	0.1063	-1.1911
6	C	3.8712	-0.8551	-0.5913
7	C	4.7299	-1.7775	0.0213
8	C	4.2054	-2.802	0.8176
9	C	2.8257	-2.9192	1.0046
10	C	1.186	1.7383	-0.1006
11	C	1.2022	2.9671	-0.7707
12	C	1.2757	4.1676	-0.0555
13	C	1.3346	4.1448	1.3391
14	C	1.3195	2.9196	2.0158
15	C	1.2462	1.725	1.2983
16	H	5.804	-1.6933	-0.1173
17	C	-1.6085	-0.7476	-0.1103

18	C	-2.2421	-0.0764	-1.1792
19	C	-3.618	0.1009	-1.214
20	C	-4.4177	-0.3755	-0.1645
21	C	-3.8145	-1.0286	0.919
22	C	-2.4289	-1.1964	0.9394
23	H	-0.0011	-2.7441	1.0998
24	H	4.2848	-0.0675	-1.2159
25	H	4.8744	-3.518	1.2866
26	H	2.4236	-3.7216	1.6182
27	H	1.1534	2.9909	-1.8564
28	H	1.2864	5.1148	-0.5877
29	H	1.3905	5.0748	1.8977
30	H	1.3646	2.8968	3.1012
31	H	1.2339	0.7786	1.8313
32	H	-1.6418	0.282	-2.0104
33	H	-4.0971	0.6073	-2.0457
34	H	-4.4031	-1.3907	1.7537
35	H	-1.9784	-1.6801	1.8011
36	O	-5.7597	-0.1507	-0.2874
37	C	-6.6241	-0.6074	0.7457
38	H	-7.6313	-0.3253	0.4367
39	H	-6.5702	-1.6974	0.8596
40	H	-6.39	-0.1275	1.7043

5b (S_0): *E*(B3LYP) = -3234.079556 hartree

Number	Atom	X	Y	Z
1	C	1.5704	-1.7648	0.5524
2	C	0.1162	-1.8631	0.6192
3	C	-0.609	-0.945	-0.07
4	As	0.5789	0.217	-1.1199
5	C	2.0558	-0.7174	-0.2574
6	C	3.4214	-0.5237	-0.4532
7	C	4.3291	-1.3797	0.1894
8	C	3.8587	-2.4223	1.0061

9	C	2.4934	-2.6214	1.1764
10	C	0.516	1.8683	-0.0541
11	O	5.6895	-1.28	0.0848
12	C	-2.0676	-0.8344	-0.1296
13	C	0.4693	3.0879	-0.7394
14	C	0.4272	4.298	-0.0376
15	C	0.4327	4.2941	1.3585
16	C	0.4799	3.0782	2.0505
17	C	0.5217	1.8746	1.346
18	C	-2.7139	-0.2582	-1.2452
19	C	-4.0967	-0.1613	-1.3163
20	C	-4.892	-0.6305	-0.2604
21	C	-4.2777	-1.1931	0.8664
22	C	-2.8857	-1.2813	0.9229
23	C	6.2356	-0.2309	-0.7048
24	O	-6.2424	-0.4899	-0.4209
25	C	-7.1014	-0.9556	0.6121
26	H	-0.3478	-2.6673	1.1884
27	H	3.7718	0.2776	-1.0939
28	H	4.5855	-3.0701	1.4853
29	H	2.1438	-3.4429	1.7968
30	H	0.461	3.0969	-1.8265
31	H	0.3888	5.2378	-0.5814
32	H	0.3982	5.2316	1.9063
33	H	0.4835	3.0699	3.137
34	H	0.557	0.9351	1.8899
35	H	-2.1157	0.0968	-2.0796
36	H	-4.5843	0.2744	-2.1825
37	H	-4.8639	-1.5474	1.7061
38	H	-2.428	-1.6921	1.818
39	H	7.3187	-0.3383	-0.6333
40	H	5.9305	-0.3196	-1.7551
41	H	5.9408	0.7538	-0.3206
42	H	-8.1165	-0.7506	0.2699
43	H	-6.983	-2.0344	0.7749

44	H	-6.9208	-0.4222	1.554

6a (S_0): *E*(B3LYP) = -3342.081199 hartree

Number	Atom	X	Y	Z
1	C	2.4997	-1.9817	0.4048
2	C	1.0502	-1.9686	0.576
3	C	0.3571	-0.9813	-0.0467
4	As	1.546	0.0957	-1.1827
5	C	3.0004	-0.956	-0.4304
6	C	4.3666	-0.8428	-0.6644
7	C	5.2491	-1.7547	-0.071
8	C	4.7585	-2.7781	0.7486
9	C	3.387	-2.9026	0.9816
10	C	1.6757	1.7438	-0.1205
11	C	-1.0921	-0.7741	-0.0009
12	C	1.6757	2.9599	-0.8137
13	C	1.7589	4.173	-0.1214
14	C	1.8442	4.1751	1.272
15	C	1.846	2.9625	1.9711
16	C	1.7631	1.7548	1.2771
17	C	-1.7662	-0.1558	-1.0735
18	C	-3.1463	0.0166	-1.0548
19	C	-3.8893	-0.4086	0.0515
20	C	-3.2392	-1.0067	1.1366
21	C	-1.859	-1.1822	1.109
22	C	-5.3834	-0.2452	0.0521
23	F	-5.7759	0.9008	-0.5616
24	F	-5.9023	-0.2233	1.3053
25	F	-6.0088	-1.2626	-0.606
26	H	0.5654	-2.7438	1.1672
27	H	4.7559	-0.0583	-1.3079
28	H	6.3174	-1.6655	-0.2454
29	H	5.4478	-3.4855	1.2004
30	H	3.0093	-3.7034	1.6122

31	H	1.6052	2.9643	-1.8984
32	H	1.7561	5.1104	-0.6704
33	H	1.9069	5.1151	1.8127
34	H	1.9115	2.9597	3.0556
35	H	1.7648	0.8186	1.8279
36	H	-1.1991	0.1667	-1.9413
37	H	-3.6448	0.4884	-1.895
38	H	-3.8085	-1.3203	2.0048
39	H	-1.3649	-1.6214	1.9698

6b (S_0): *E*(B3LYP) = -3456.610798 hartree

Number	Atom	X	Y	Z
1	C	2.0658	-1.7725	0.5688
2	C	0.6154	-1.8422	0.6899
3	C	-0.116	-0.916	0.0172
4	As	1.0508	0.2111	-1.0914
5	C	2.5389	-0.7413	-0.269
6	C	3.9003	-0.5665	-0.5041
7	C	4.815	-1.427	0.1232
8	C	4.3553	-2.4568	0.9641
9	C	2.9944	-2.6344	1.1784
10	C	1.0575	1.8787	-0.0507
11	O	6.1702	-1.3478	-0.0218
12	C	-1.5738	-0.7893	0.0079
13	C	1.0309	3.0846	-0.7608
14	C	1.0356	4.3091	-0.0833
15	C	1.0675	4.3325	1.3122
16	C	1.0952	3.13	2.0281
17	C	1.0915	1.9112	1.3486
18	C	-2.242	-0.2037	-1.0865
19	C	-3.6282	-0.0849	-1.1083
20	C	-4.3851	-0.5314	-0.0207
21	C	-3.7424	-1.1018	1.0846
22	C	-2.3572	-1.2244	1.0973

23	C	6.7106	-0.3264	-0.8528
24	C	-5.8845	-0.4498	-0.0612
25	F	-6.3266	0.5871	-0.8172
26	F	-6.4439	-1.5753	-0.5918
27	F	-6.4281	-0.3025	1.1744
28	H	0.1576	-2.6324	1.2831
29	H	4.2436	0.2232	-1.1627
30	H	5.0882	-3.1085	1.4283
31	H	2.6518	-3.4431	1.819
32	H	1.0009	3.0722	-1.8474
33	H	1.0121	5.2385	-0.6453
34	H	1.0682	5.2811	1.8414
35	H	1.1189	3.1438	3.1142
36	H	1.1123	0.9826	1.9116
37	H	-1.6642	0.1386	-1.9395
38	H	-4.1206	0.3619	-1.9654
39	H	-4.3238	-1.4352	1.9378
40	H	-1.8718	-1.6391	1.9749
41	H	7.7927	-0.4556	-0.815
42	H	6.3672	-0.4323	-1.8893
43	H	6.4492	0.6716	-0.4797

7a (S_0): *E*(B3LYP) = -3138.999251 hartree

Number	Atom	X	Y	Z
1	C	2.3229	-1.9504	0.3596
2	C	0.8722	-1.9904	0.5146
3	C	0.1487	-1.013	-0.0924
4	As	1.3163	0.1299	-1.1872
5	C	2.7999	-0.896	-0.4543
6	C	4.1626	-0.7376	-0.6793
7	C	5.0715	-1.6331	-0.0995
8	C	4.6063	-2.6834	0.7001
9	C	3.2374	-2.8535	0.9224
10	C	1.3939	1.7445	-0.0667

11	C	-1.301	-0.8365	-0.0504
12	C	1.3902	2.9856	-0.7143
13	C	1.4406	4.1743	0.0224
14	C	1.4954	4.1276	1.4166
15	C	1.4991	2.8904	2.0711
16	C	1.4487	1.7078	1.3319
17	C	-1.9891	-0.1483	-1.0677
18	C	-3.3716	-0.0054	-1.0615
19	C	-4.1592	-0.5545	-0.0222
20	C	-3.4693	-1.2164	1.0233
21	C	-2.0871	-1.3494	1.0002
22	N	-5.5449	-0.4453	-0.0248
23	C	-6.2898	-0.8229	1.1666
24	C	-6.1788	0.4894	-0.9431
25	H	0.4098	-2.7914	1.089
26	H	4.5296	0.0703	-1.3072
27	H	6.1375	-1.5083	-0.2666
28	H	5.3137	-3.3786	1.1436
29	H	2.8819	-3.677	1.537
30	H	1.3438	3.028	-1.7996
31	H	1.4366	5.131	-0.4929
32	H	1.5334	5.0484	1.9919
33	H	1.5407	2.8488	3.1561
34	H	1.45	0.7519	1.8476
35	H	-1.4269	0.2676	-1.8992
36	H	-3.8363	0.5329	-1.8781
37	H	-4.0111	-1.62	1.8697
38	H	-1.6032	-1.8471	1.8358
39	H	-6.1038	-1.87	1.4269
40	H	-6.0409	-0.2012	2.0422
41	H	-7.3574	-0.7208	0.9652
42	H	-5.8647	1.5318	-0.7727
43	H	-5.954	0.2306	-1.9831
44	H	-7.2613	0.4313	-0.8187

7b (S_0): *E*(B3LYP) = -3253.527947 hartree

Number	Atom	X	Y	Z
1	C	1.8784	-1.7679	0.5305
2	C	0.4279	-1.8848	0.6346
3	C	-0.3273	-0.9674	-0.0244
4	As	0.8193	0.2207	-1.092
5	C	2.3305	-0.71	-0.2851
6	C	3.6881	-0.499	-0.5154
7	C	4.6229	-1.3479	0.0972
8	C	4.1864	-2.4005	0.9193
9	C	2.8281	-2.6166	1.1248
10	C	0.776	1.8551	0.0025
11	C	-1.7853	-0.8695	-0.0439
12	C	0.7467	3.0853	-0.6648
13	C	0.719	4.2858	0.0542
14	C	0.721	4.2616	1.4501
15	C	0.75	3.0352	2.1241
16	C	0.7775	1.8411	1.4025
17	C	-2.4688	-0.2464	-1.1049
18	C	-3.8558	-0.1613	-1.1456
19	C	-4.653	-0.7054	-0.1116
20	C	-3.9699	-1.3039	0.9752
21	C	-2.5833	-1.3824	0.9978
22	N	-6.0427	-0.6529	-0.159
23	C	-6.806	-1.0166	1.0248
24	C	-6.6821	0.2386	-1.1156
25	O	5.9798	-1.2314	-0.0434
26	C	6.4911	-0.1734	-0.8434
27	H	-0.0105	-2.699	1.2096
28	H	4.0117	0.3107	-1.1595
29	H	4.9332	-3.0428	1.3749
30	H	2.5049	-3.4458	1.7494
31	H	0.7404	3.11	-1.7516
32	H	0.6946	5.2339	-0.4761

33	H	0.6977	5.1914	2.0115
34	H	0.7504	3.011	3.2105
35	H	0.7977	0.8932	1.9325
36	H	-1.8981	0.1671	-1.9321
37	H	-4.3155	0.3291	-1.9946
38	H	-4.5209	-1.702	1.8182
39	H	-2.1065	-1.8309	1.8647
40	H	-6.5837	-2.044	1.3307
41	H	-6.6103	-0.3523	1.8828
42	H	-7.8705	-0.9689	0.7893
43	H	-6.4138	1.2958	-0.9576
44	H	-6.4147	-0.0316	-2.1425
45	H	-7.765	0.1406	-1.0241
46	H	7.577	-0.2684	-0.8036
47	H	6.1571	-0.2611	-1.8851
48	H	6.1964	0.8066	-0.4471

4a-AuCl (S_0): *E*(B3LYP) = -1373.394855 hartree

Number	Atom	X	Y	Z
1	C	-0.95136	-2.12459	-0.61069
2	C	-1.97832	-1.86733	-1.54405
3	C	-2.30046	-0.45299	-1.74684
4	C	-0.94395	-0.27461	1.903276
5	C	-0.53064	-3.41817	-0.33159
6	C	-1.15697	-4.48857	-0.98443
7	C	-2.17641	-4.24884	-1.90965
8	C	-2.58833	-2.94528	-2.19705
9	H	-3.06733	-0.17596	-2.4676
10	C	-2.28866	-0.53153	2.198421
11	C	-2.74105	-0.41397	3.512375
12	C	-1.85618	-0.04106	4.528618
13	C	-0.5171	0.215005	4.23219
14	C	-0.05637	0.09899	2.91776
15	H	0.271047	-3.60433	0.377803

16	H	-0.84343	-5.5066	-0.77252
17	H	-2.65143	-5.08459	-2.41582
18	H	-3.37572	-2.76646	-2.92485
19	H	-2.97991	-0.81986	1.411269
20	H	-3.78403	-0.6126	3.74326
21	H	-2.21285	0.049719	5.550905
22	H	0.172572	0.505438	5.019668
23	H	0.986594	0.298717	2.6851
24	C	-1.60823	0.477982	-1.04692
25	C	-1.79835	1.932317	-1.0663
26	C	-0.73392	2.816747	-0.80881
27	C	-3.06599	2.480023	-1.34858
28	C	-0.92591	4.196722	-0.85242
29	H	0.257831	2.424255	-0.60024
30	C	-3.25399	3.858551	-1.39353
31	H	-3.91033	1.816379	-1.51161
32	C	-2.18441	4.723864	-1.1468
33	H	-0.08674	4.859132	-0.65972
34	H	-4.2407	4.259057	-1.60999
35	H	-2.33341	5.799513	-1.17768
36	As	-0.27557	-0.43729	0.074663
37	Au	2.088397	0.052317	-0.18105
38	Cl	4.343985	0.52331	-0.39053

4a (S_1): *E*(B3LYP) = -777.213419 hartree

Number	Atom	X	Y	Z
1	As	0.351211	0.044094	-0.97757
2	C	1.774667	-1.18523	-0.52413
3	C	1.26162	-1.96884	0.558924
4	C	-0.12949	-1.81535	0.869187
5	C	0.761915	1.753326	-0.1291
6	C	3.083904	-1.25769	-0.96366
7	C	3.971518	-2.13948	-0.32134
8	C	3.512646	-2.88283	0.776487
9	C	2.198035	-2.7933	1.227665
10	H	-0.54718	-2.32297	1.735535
11	C	2.082387	2.23698	-0.11773
12	C	2.361591	3.471376	0.461789
13	C	1.325711	4.235995	1.011539
14	C	0.008627	3.763997	0.987562
15	C	-0.28098	2.531139	0.407748
16	H	3.425944	-0.65675	-1.80334
17	H	4.992638	-2.24254	-0.67393
18	H	4.201046	-3.54771	1.29308
19	H	1.880094	-3.36135	2.098766
20	H	2.887576	1.633486	-0.52738
21	H	3.383859	3.837932	0.492064
22	H	1.545974	5.201227	1.458966
23	H	-0.7902	4.357721	1.422651
24	H	-1.30197	2.161871	0.392003
25	C	-0.93303	-0.98969	0.068421
26	C	-2.34341	-0.7778	0.037053
27	C	-2.96863	0.20158	-0.78647
28	C	-3.21608	-1.57945	0.834898
29	C	-4.34633	0.370984	-0.80851
30	H	-2.35333	0.828363	-1.43086
31	C	-4.59003	-1.39373	0.810755
32	H	-2.79395	-2.35941	1.461058
33	C	-5.17955	-0.41661	-0.0039

34	H	-4.77704	1.127303	-1.46086
35	H	-5.21771	-2.02656	1.434604
36	H	-6.25627	-0.27797	-0.01556

4b (S_1): *E*(B3LYP) = -891.738482 hartree

Number	Atom	X	Y	Z
1	As	-0.16054	0.231563	-1.21097
2	C	1.510365	-0.43327	-0.44664
3	C	1.285549	-1.51982	0.496906
4	C	-0.05593	-1.88475	0.676307
5	C	-0.51107	1.8989	-0.07497
6	C	2.801389	-0.01584	-0.72887
7	C	3.89624	-0.6333	-0.10297
8	C	3.695958	-1.69566	0.829475
9	C	2.419398	-2.12717	1.114398
10	H	-0.32677	-2.72922	1.302748
11	C	-0.62023	1.874816	1.319898
12	C	-0.81805	3.060172	2.031732
13	C	-0.90709	4.27918	1.353189
14	C	-0.799	4.309904	-0.03865
15	C	-0.60026	3.12151	-0.748
16	H	3.004061	0.787485	-1.43186
17	H	4.543168	-2.16602	1.314782
18	H	2.268631	-2.93666	1.824507
19	H	-0.55671	0.928461	1.851585
20	H	-0.90448	3.034981	3.115841
21	H	-1.0614	5.201194	1.908177
22	H	-0.87285	5.2559	-0.57043
23	H	-0.51882	3.148584	-1.834
24	C	-1.01796	-1.13065	-0.06342
25	C	-2.43101	-1.3553	-0.0283
26	C	-3.32574	-0.60036	-0.84276
27	C	-3.01824	-2.33277	0.835917
28	C	-4.6943	-0.80641	-0.8011

29	H	-2.91906	0.15073	-1.51474
30	C	-4.39144	-2.52773	0.873686
31	H	-2.38218	-2.92784	1.482531
32	C	-5.24325	-1.77232	0.058499
33	H	-5.34591	-0.21368	-1.43774
34	H	-4.80726	-3.27609	1.543966
35	H	-6.31762	-1.93017	0.091433
36	O	5.119224	-0.15729	-0.44756
37	C	6.283325	-0.72964	0.132998
38	H	7.126106	-0.1879	-0.2993
39	H	6.291462	-0.60426	1.223286
40	H	6.371853	-1.79579	-0.11201

5a (S_1): *E*(B3LYP) = -891.739034 hartree

Number	Atom	X	Y	Z
1	C	2.403206	-1.07783	-0.45671
2	C	1.825455	-2.04194	0.467292
3	C	0.435466	-1.94136	0.620285
4	C	-0.21776	-0.91449	-0.12672
5	As	1.061468	0.106495	-1.23002
6	C	3.77114	-1.11766	-0.72687
7	C	4.583883	-2.06195	-0.10033
8	C	4.031317	-3.00203	0.812816
9	C	2.681274	-2.99907	1.089772
10	C	1.283481	1.78211	-0.06639
11	C	1.39243	3.010503	-0.72506
12	C	1.564839	4.193549	0.000921
13	C	1.631677	4.150135	1.394706
14	C	1.525734	2.924519	2.059331
15	C	1.353133	1.745473	1.330763
16	H	5.65029	-2.08209	-0.30891
17	C	-1.62782	-0.68786	-0.11999
18	C	-2.21885	0.374815	-0.8729
19	C	-3.57609	0.603119	-0.87225

20	C	-4.43788	-0.21595	-0.10687
21	C	-3.89678	-1.26886	0.65201
22	C	-2.5291	-1.49672	0.642653
23	H	-0.10616	-2.6409	1.251501
24	H	4.211928	-0.40735	-1.42297
25	H	4.682722	-3.72925	1.289854
26	H	2.256107	-3.72332	1.781243
27	H	1.341522	3.047339	-1.81268
28	H	1.645974	5.145393	-0.51935
29	H	1.76665	5.067374	1.962544
30	H	1.578603	2.889816	3.145338
31	H	1.270527	0.795142	1.85272
32	H	-1.5743	1.023051	-1.45946
33	H	-4.01274	1.413886	-1.44688
34	H	-4.53774	-1.91066	1.246258
35	H	-2.14024	-2.32037	1.231051
36	O	-5.75431	0.098821	-0.17013
37	C	-6.68205	-0.67383	0.580687
38	H	-7.66259	-0.24011	0.37895
39	H	-6.67439	-1.72447	0.263655
40	H	-6.47032	-0.61641	1.655969

5b (S_1): *E*(B3LYP) = -1006.265296 hartree

Number	Atom	X	Y	Z
1	C	1.493113	-1.77509	0.611973
2	C	0.096058	-1.82932	0.697485
3	C	-0.62224	-0.88046	-0.08708
4	As	0.588494	0.255036	-1.15457
5	C	2.00848	-0.77125	-0.30583
6	C	3.383581	-0.64664	-0.50831
7	C	4.262147	-1.49042	0.180082
8	C	3.769593	-2.47831	1.089516
9	C	2.419985	-2.61794	1.294342
10	C	0.518898	1.979316	-0.0122

11	O	5.614312	-1.46579	0.063305
12	C	-2.04936	-0.78961	-0.14131
13	C	0.722779	3.192061	-0.67715
14	C	0.746108	4.397325	0.031817
15	C	0.571173	4.392086	1.417345
16	C	0.370884	3.182165	2.088978
17	C	0.345585	1.981106	1.375947
18	C	-2.70582	0.177625	-0.9615
19	C	-4.07842	0.284231	-1.01064
20	C	-4.88861	-0.57214	-0.23395
21	C	-4.28165	-1.53588	0.5888
22	C	-2.89837	-1.64001	0.628917
23	C	6.206626	-0.51239	-0.80803
24	O	-6.22743	-0.3831	-0.35215
25	C	-7.10287	-1.20802	0.403717
26	H	-0.39591	-2.58619	1.302115
27	H	3.762915	0.101753	-1.1964
28	H	4.494689	-3.10282	1.601024
29	H	2.048139	-3.37289	1.983203
30	H	0.859202	3.199122	-1.75849
31	H	0.896385	5.337477	-0.49478
32	H	0.590468	5.326588	1.972756
33	H	0.233105	3.177486	3.168292
34	H	0.184331	1.042636	1.901784
35	H	-2.10405	0.850281	-1.56572
36	H	-4.56442	1.024242	-1.63872
37	H	-4.88145	-2.2049	1.195898
38	H	-2.45862	-2.39345	1.273248
39	H	7.28381	-0.67249	-0.73845
40	H	5.87902	-0.66326	-1.84467
41	H	5.966113	0.512457	-0.49792
42	H	-8.11284	-0.87971	0.152985
43	H	-6.98604	-2.26615	0.136188
44	H	-6.93631	-1.08585	1.481756

6a (S_1): *E*(B3LYP) = -1114.249104 hartree

Number	Atom	X	Y	Z
1	C	2.432171	-1.99825	0.441902
2	C	1.042684	-1.96998	0.623666
3	C	0.323198	-0.963	-0.09589
4	As	1.534336	0.113167	-1.23985
5	C	2.954946	-0.99161	-0.47063
6	C	4.319166	-0.94121	-0.7423
7	C	5.187658	-1.8502	-0.13505
8	C	4.690596	-2.83909	0.758058
9	C	3.345601	-2.92154	1.040761
10	C	1.708683	1.772885	-0.09582
11	C	-1.0873	-0.77079	-0.04275
12	C	1.707083	3.010703	-0.74801
13	C	1.835735	4.195539	-0.01761
14	C	1.968191	4.146057	1.371905
15	C	1.972023	2.912376	2.028884
16	C	1.844052	1.72959	1.297875
17	C	-1.7393	0.224163	-0.83498
18	C	-3.10651	0.408064	-0.78873
19	C	-3.90204	-0.38547	0.062032
20	C	-3.29393	-1.36542	0.860643
21	C	-1.92449	-1.55851	0.815647
22	C	-5.39051	-0.21363	0.064738
23	F	-5.74775	1.082588	-0.09328
24	F	-5.95272	-0.6543	1.213134
25	F	-5.98252	-0.89936	-0.94634
26	H	0.54518	-2.71602	1.236181
27	H	4.714569	-0.196	-1.42852
28	H	6.252166	-1.80873	-0.34856
29	H	5.385002	-3.53742	1.217077
30	H	2.96642	-3.6797	1.721461
31	H	1.60356	3.053017	-1.83093
32	H	1.831246	5.153987	-0.53098

33	H	2.067998	5.066116	1.941884
34	H	2.074691	2.873112	3.110654
35	H	1.846015	0.773338	1.814397
36	H	-1.14118	0.852229	-1.48949
37	H	-3.57305	1.174468	-1.39935
38	H	-3.90472	-1.9702	1.523195
39	H	-1.48022	-2.31712	1.450461

6b (S_1): *E*(B3LYP) = -1228.777319 hartree

Number	Atom	X	Y	Z
1	C	2.010184	-1.78067	0.608474
2	C	0.612059	-1.83495	0.747414
3	C	-0.13264	-0.88754	-0.01278
4	As	1.045369	0.240513	-1.1349
5	C	2.504365	-0.76921	-0.30837
6	C	3.867687	-0.63156	-0.54607
7	C	4.770614	-1.47912	0.11269
8	C	4.300955	-2.48196	1.016983
9	C	2.958178	-2.63238	1.254358
10	C	1.069905	1.939492	-0.01979
11	O	6.115202	-1.44485	-0.03392
12	C	-1.55857	-0.7759	-0.02074
13	C	1.210592	3.151964	-0.70311
14	C	1.262037	4.35964	-0.00053
15	C	1.173377	4.358048	1.392913
16	C	1.032258	3.149412	2.081023
17	C	0.981461	1.944263	1.37727
18	C	-2.23289	0.15202	-0.8682
19	C	-3.60993	0.266065	-0.8723
20	C	-4.39138	-0.53734	-0.02009
21	C	-3.75925	-1.45546	0.830746
22	C	-2.38003	-1.5771	0.834569
23	C	6.689169	-0.47712	-0.90564
24	C	-5.88535	-0.44753	-0.07066

25	F	-6.30777	0.817502	-0.3057
26	F	-6.40999	-1.21441	-1.0614
27	F	-6.46117	-0.86076	1.082081
28	H	0.141427	-2.59949	1.357599
29	H	4.224988	0.124547	-1.23729
30	H	5.040584	-3.11224	1.500087
31	H	2.607542	-3.39729	1.942367
32	H	1.27503	3.157156	-1.79022
33	H	1.366433	5.29853	-0.53922
34	H	1.211519	5.295416	1.94196
35	H	0.960007	3.147573	3.166143
36	H	0.866736	1.007495	1.916751
37	H	-1.64838	0.784946	-1.53049
38	H	-4.09351	0.984723	-1.52627
39	H	-4.35851	-2.06932	1.495682
40	H	-1.91851	-2.28705	1.512164
41	H	7.767273	-0.63542	-0.8566
42	H	6.342288	-0.61885	-1.93683
43	H	6.449913	0.541727	-0.57674

7a (S_1): *E*(B3LYP) = -911.189888 hartree

Number	Atom	X	Y	Z
1	C	2.209567	-2.0008	0.433398
2	C	0.81229	-1.96297	0.606347
3	C	0.106379	-0.96279	-0.10681
4	As	1.315419	0.122934	-1.22009
5	C	2.723943	-1.00821	-0.49072
6	C	4.08659	-0.9892	-0.79223
7	C	4.952798	-1.90125	-0.19006
8	C	4.46026	-2.86692	0.727819
9	C	3.1145	-2.92123	1.031316
10	C	1.46621	1.803533	-0.0379
11	C	-1.31872	-0.79734	-0.06726
12	C	1.593157	3.035232	-0.68702

13	C	1.730261	4.217546	0.048152
14	C	1.744433	4.170431	1.443274
15	C	1.620616	2.941529	2.09915
16	C	1.48269	1.764024	1.360622
17	C	-1.96256	0.297845	-0.71326
18	C	-3.32949	0.477381	-0.68491
19	C	-4.17621	-0.43271	0.008739
20	C	-3.55344	-1.52898	0.662872
21	C	-2.18383	-1.70205	0.622635
22	N	-5.54228	-0.25228	0.047009
23	C	-6.38349	-1.1841	0.780729
24	C	-6.15466	0.87447	-0.63967
25	H	0.315016	-2.68622	1.248843
26	H	4.481356	-0.25556	-1.49219
27	H	6.014518	-1.87359	-0.42129
28	H	5.15022	-3.56891	1.188582
29	H	2.734902	-3.66841	1.725599
30	H	1.583704	3.075028	-1.77596
31	H	1.82502	5.171727	-0.46602
32	H	1.852803	5.086565	2.018836
33	H	1.632636	2.903522	3.186488
34	H	1.384855	0.810787	1.874932
35	H	-1.35298	1.025754	-1.24034
36	H	-3.75152	1.33577	-1.19393
37	H	-4.15249	-2.2534	1.202282
38	H	-1.76032	-2.56519	1.124655
39	H	-6.30694	-2.20256	0.375373
40	H	-6.11127	-1.22011	1.844488
41	H	-7.42381	-0.86556	0.706085
42	H	-5.79698	1.834121	-0.24179
43	H	-5.94332	0.852384	-1.71726
44	H	-7.23603	0.832326	-0.50473

7b (S_1): *E*(B3LYP) = -1025.714540 hartree

Number	Atom	X	Y	Z
1	C	1.835322	-1.77413	0.58102
2	C	0.437396	-1.86332	0.680914
3	C	-0.31312	-0.91943	-0.06433
4	As	0.852822	0.258941	-1.13532
5	C	2.308039	-0.74984	-0.33145
6	C	3.678981	-0.58947	-0.55241
7	C	4.587124	-1.41839	0.112455
8	C	4.134186	-2.42529	1.018635
9	C	2.788989	-2.59897	1.240203
10	C	0.704624	1.973979	0.034521
11	C	-1.74506	-0.85692	-0.08035
12	C	0.879537	3.201258	-0.61245
13	C	0.881131	4.396775	0.113031
14	C	0.719307	4.368413	1.500287
15	C	0.552818	3.144098	2.155356
16	C	0.546074	1.953412	1.424683
17	C	-2.44134	0.127823	-0.83804
18	C	-3.81714	0.221025	-0.8509
19	C	-4.62158	-0.6753	-0.09392
20	C	-3.94628	-1.66537	0.668122
21	C	-2.56794	-1.75073	0.669549
22	N	-5.9964	-0.58506	-0.1009
23	C	-6.79465	-1.51279	0.683968
24	C	-6.66034	0.444962	-0.88443
25	O	5.939577	-1.3597	-0.02803
26	C	6.488547	-0.38161	-0.89744
27	H	-0.02606	-2.64131	1.282892
28	H	4.028909	0.175773	-1.23777
29	H	4.880818	-3.0364	1.515092
30	H	2.445734	-3.37091	1.925748
31	H	1.010819	3.226385	-1.69451
32	H	1.005136	5.34774	-0.40142
33	H	0.725013	5.29494	2.069431
34	H	0.426427	3.120635	3.23609

35	H	0.41007	1.003743	1.937794
36	H	-1.86824	0.836775	-1.42798
37	H	-4.27963	0.996834	-1.44942
38	H	-4.51076	-2.37376	1.263264
39	H	-2.10432	-2.5271	1.2687
40	H	-6.62905	-2.55302	0.371445
41	H	-6.56395	-1.43896	1.755788
42	H	-7.85194	-1.28206	0.547707
43	H	-6.36472	1.452748	-0.56213
44	H	-6.43218	0.349169	-1.95476
45	H	-7.73977	0.35157	-0.75858
46	H	7.571246	-0.51273	-0.8513
47	H	6.145877	-0.52699	-1.93039
48	H	6.227933	0.633765	-0.57154

4a-AuCl (S_1): *E*(B3LYP) = -1373.274151 hartree

Number	Atom	X	Y	Z
1	C	-1.14128	-2.03263	-0.58321
2	C	-2.32355	-1.71548	-1.37275
3	C	-2.60097	-0.34766	-1.50402
4	C	-0.73926	-0.24991	2.012227
5	C	-0.72202	-3.35511	-0.44521
6	C	-1.45822	-4.3753	-1.04563
7	C	-2.6273	-4.08591	-1.80444
8	C	-3.0508	-2.78551	-1.9721
9	H	-3.42144	-0.00397	-2.12588
10	C	-2.06563	-0.24615	2.457538
11	C	-2.33722	-0.15087	3.82312
12	C	-1.28647	-0.06547	4.741517
13	C	0.036571	-0.07313	4.295227
14	C	0.312523	-0.16673	2.928304
15	H	0.171592	-3.59434	0.125114
16	H	-1.1357	-5.40682	-0.93639
17	H	-3.18125	-4.90117	-2.2601

18	H	-3.93494	-2.56078	-2.56347
19	H	-2.88358	-0.31169	1.744216
20	H	-3.36686	-0.14306	4.171313
21	H	-1.50043	0.006978	5.804495
22	H	0.854352	-0.00358	5.007639
23	H	1.342294	-0.16748	2.574853
24	C	-1.72102	0.558948	-0.83607
25	C	-1.80364	1.984929	-0.89232
26	C	-0.84048	2.812677	-0.23932
27	C	-2.85988	2.645231	-1.59828
28	C	-0.9245	4.1929	-0.29445
29	H	-0.01944	2.351698	0.301409
30	C	-2.93789	4.027645	-1.63885
31	H	-3.61408	2.057104	-2.10939
32	C	-1.97398	4.813551	-0.99167
33	H	-0.17255	4.796295	0.205496
34	H	-3.75077	4.504031	-2.17985
35	H	-2.03799	5.897129	-1.02928
36	As	-0.31624	-0.43233	0.07859
37	Au	2.054012	-0.03233	-0.33435
38	Cl	4.306452	0.352055	-0.7734

8 (S_1): *E*(B3LYP) = -699.788527 hartree

Number	Atom	X	Y	Z
1	As	-0.36339	0.000231	-1.40781
2	C	0.798247	1.304468	-0.53612
3	C	1.834291	0.704214	0.320915
4	C	1.834301	-0.70423	0.320707
5	C	0.798164	-1.30426	-0.53638
6	C	-1.9844	-0.00013	-0.10003
7	C	0.75226	2.694352	-0.66316
8	C	1.65791	3.499751	0.022818
9	C	2.657245	2.926702	0.870332
10	C	2.744731	1.562404	1.012656

11	C	2.744793	-1.56261	1.012143
12	C	2.657232	-2.92688	0.86953
13	C	1.657773	-3.4997	0.022013
14	C	0.752112	-2.69411	-0.66373
15	C	-1.85829	-0.00114	1.294056
16	C	-2.99486	-0.0012	2.106856
17	C	-4.26759	-0.00025	1.528573
18	C	-4.40123	0.000751	0.137759
19	C	-3.26033	0.000819	-0.67078
20	H	0.000215	3.156908	-1.29789
21	H	1.60651	4.580289	-0.08081
22	H	3.348521	3.577778	1.396908
23	H	3.510174	1.129683	1.651139
24	H	3.510346	-1.13006	1.65061
25	H	3.348553	-3.57809	1.395871
26	H	1.606285	-4.58022	-0.08181
27	H	-8.2E-06	-3.1565	-1.29849
28	H	-0.87158	-0.00189	1.751933
29	H	-2.89093	-0.00198	3.189859
30	H	-5.15234	-0.0003	2.1604
31	H	-5.3911	0.00147	-0.31367
32	H	-3.36709	0.001608	-1.7554

10 (S_1): *E*(B3LYP) = -854.633720 hartree

Number	Atom	X	Y	Z
1	C	-0.6949	-2.10216	1.026187
2	C	0.694904	-2.10216	1.026187
3	C	-1.33703	-1.17646	0.151388
4	C	1.337027	-1.17646	0.151388
5	As	-1E-07	-0.20477	-0.91205
6	H	-1.25253	-2.80051	1.643528
7	H	1.252531	-2.80051	1.643528
8	C	-2.75245	-1.01538	0.001298
9	C	2.752448	-1.01538	0.001297

10	C	-3E-07	1.606231	0.021153
11	C	5E-07	1.741586	1.413746
12	C	-1.2E-06	2.751062	-0.78149
13	C	-1.5E-06	4.023042	-0.20027
14	C	2E-07	3.010731	1.996381
15	C	-8E-07	4.152552	1.189764
16	H	-1.7E-06	2.65325	-1.86619
17	H	-2.2E-06	4.909262	-0.83061
18	H	1.3E-06	0.855798	2.044072
19	H	8E-07	3.110921	3.079335
20	H	-1E-06	5.139898	1.644509
21	C	-3.68649	-1.7818	0.761692
22	C	-3.29537	-0.06953	-0.91564
23	C	-4.66377	0.089328	-1.06908
24	C	-5.05436	-1.61348	0.603794
25	C	-5.55791	-0.68001	-0.31131
26	H	-2.61758	0.542843	-1.50425
27	H	-5.04266	0.819833	-1.7791
28	H	-3.32402	-2.51225	1.477441
29	H	-5.73938	-2.21366	1.197468
30	H	-6.63011	-0.5507	-0.42955
31	C	3.686495	-1.7818	0.761692
32	C	3.295371	-0.06953	-0.91564
33	C	4.663772	0.089328	-1.06908
34	C	5.054362	-1.61348	0.603794
35	C	5.557913	-0.68001	-0.31131
36	H	2.617577	0.542843	-1.50425
37	H	5.042659	0.819833	-1.7791
38	H	3.324019	-2.51224	1.477442
39	H	5.739377	-2.21366	1.197468
40	H	6.630108	-0.5507	-0.42955