ESI for:

Beyond simple hetero Diels-Alder Cycloadditions. A New Type of Element-Ligand Cooperativity at *N,C,N*-coordinated Arsinidene and Stibinidene Centres in the Reaction with Electron Deficient Alkyne.

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1) NMR spectra of studied compounds.

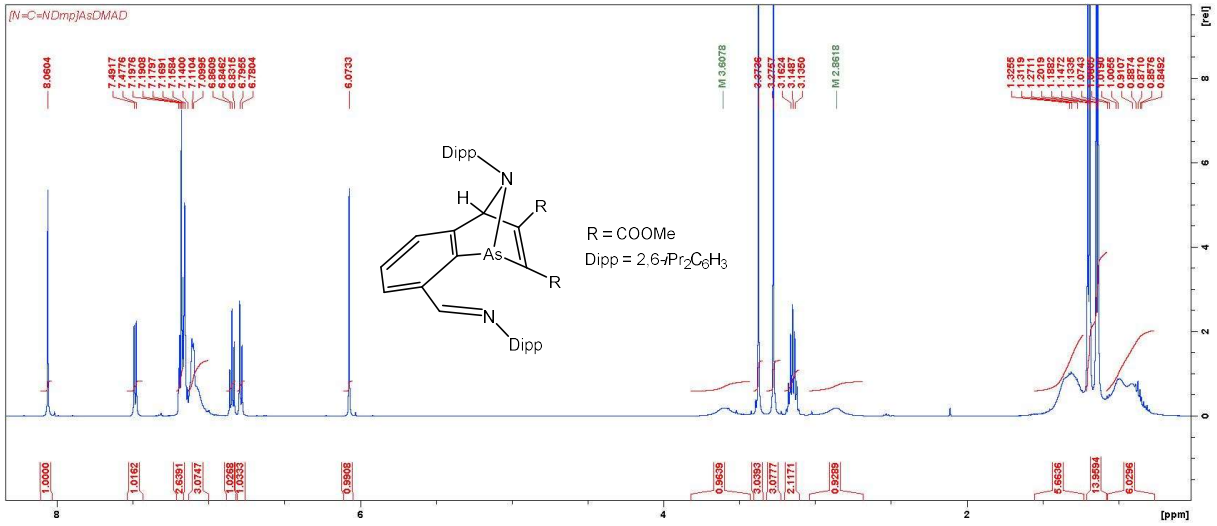


Figure S1: ^{1}H NMR spectrum of **2-As** in C_6D_6 (500 MHz).

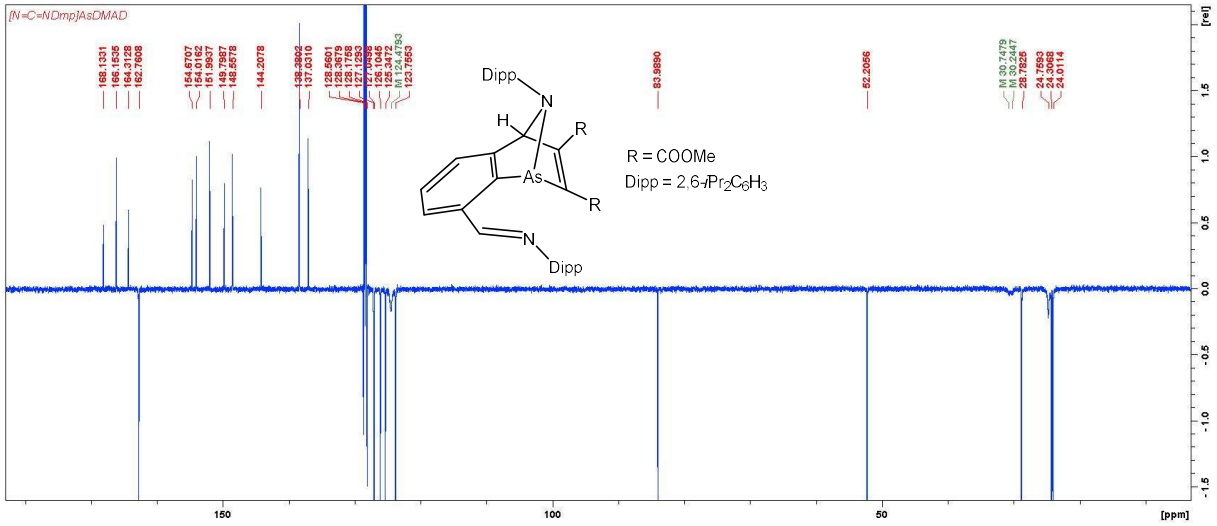


Figure S2: $^{13}C\{^{1}H\}$ NMR spectrum of **2-As** in C_6D_6 (125.6 MHz).

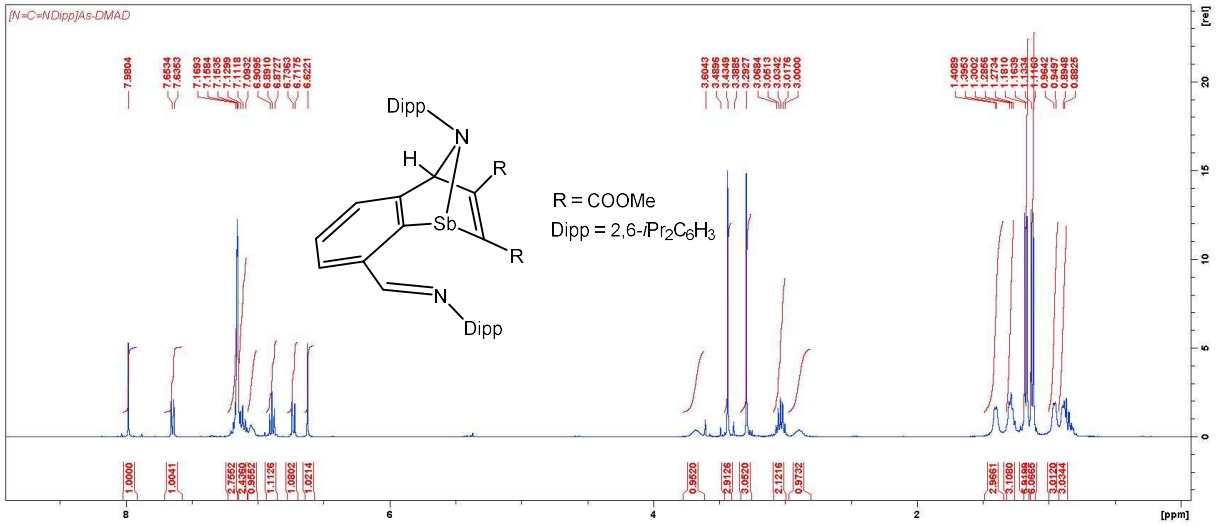


Figure S3: ^{1}H NMR spectrum of **2-Sb** in C_6D_6 (400 MHz).

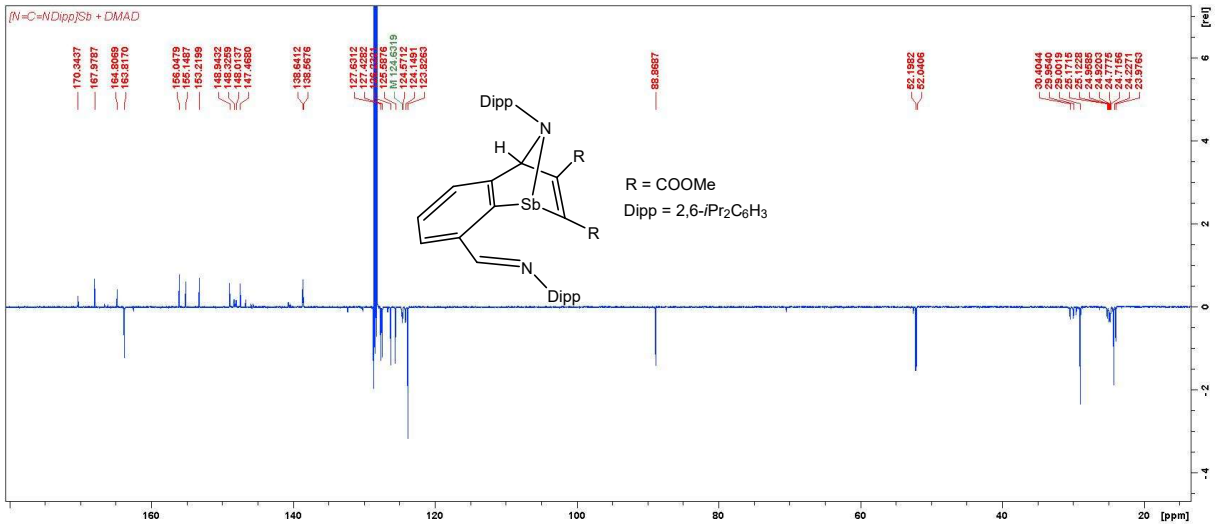


Figure S4: ^{13}C{^{1}H} NMR spectrum of **2-Sb** in C_6D_6 (125.6 MHz).

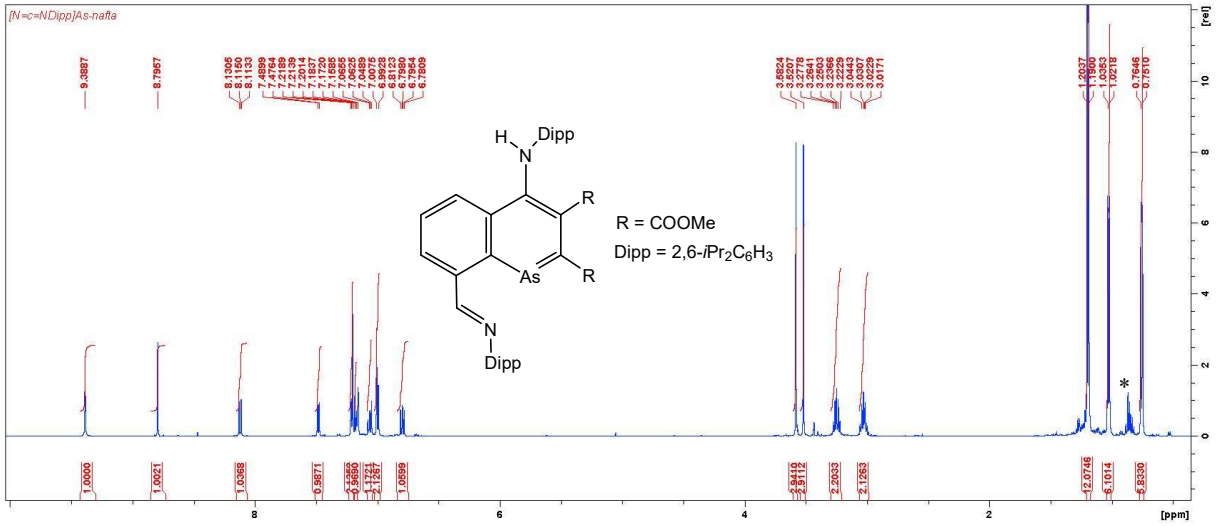


Figure S5: ^{1}H NMR spectrum of **3-As** in C_6D_6 (500 MHz). *denotes traces of hexane solvent.

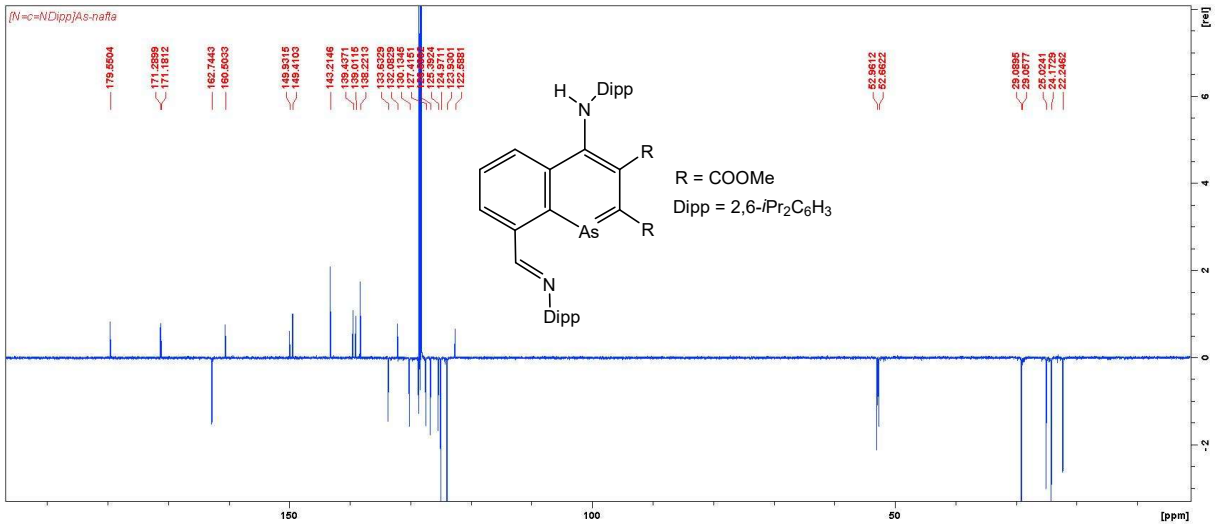


Figure S6: $^{13}C\{^{1}H\}$ NMR spectrum of **3-As** in C_6D_6 (125.6 MHz).

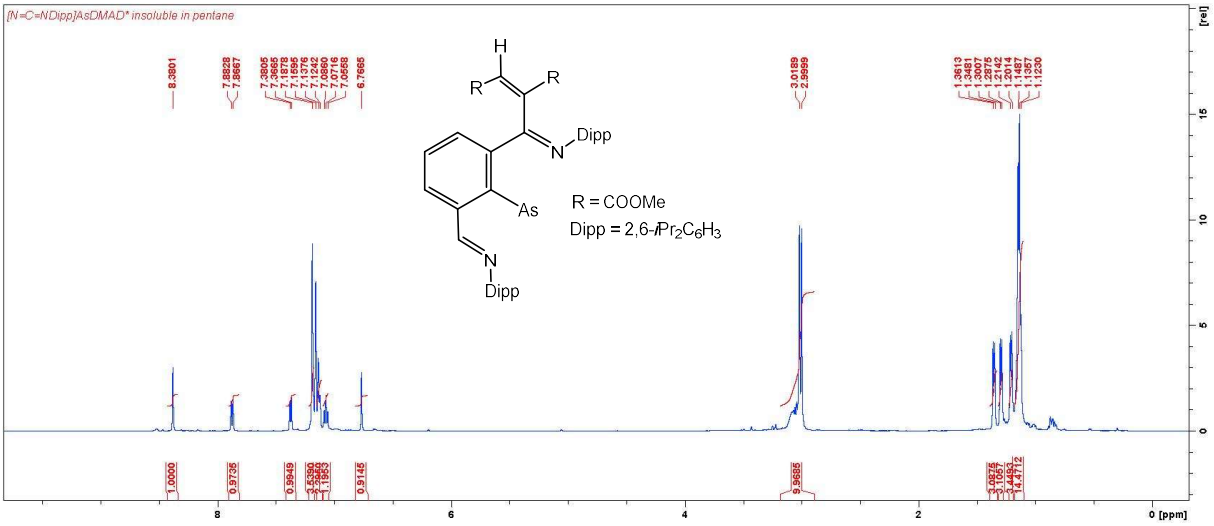


Figure S7: ^{1}H NMR spectrum of **4-As** in C_6D_6 (500 MHz).

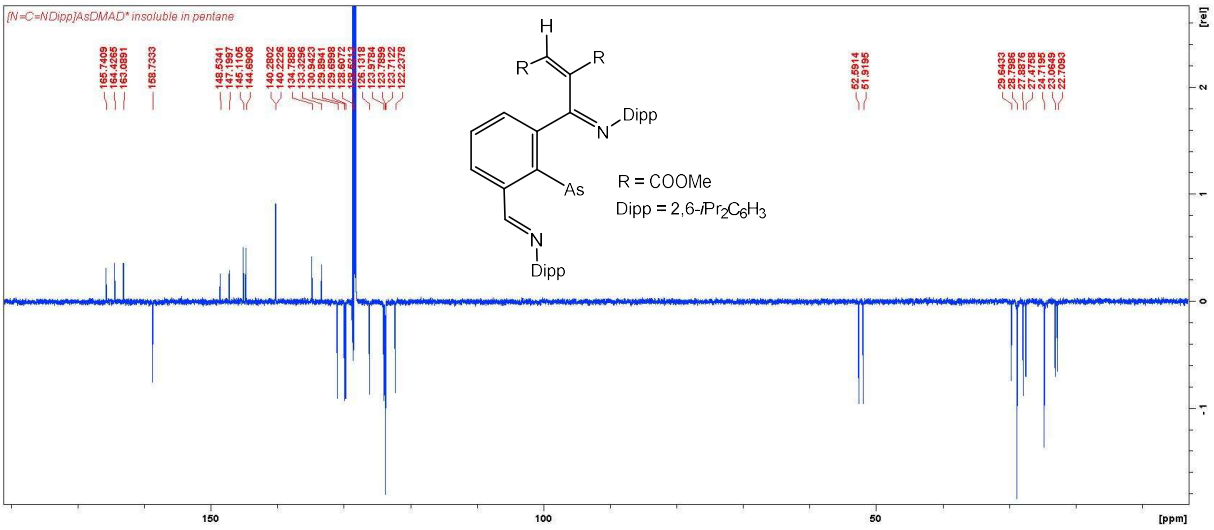


Figure S8: ^{13}C{^{1}H} NMR spectrum of **4-As** in C_6D_6 (125.6 MHz).

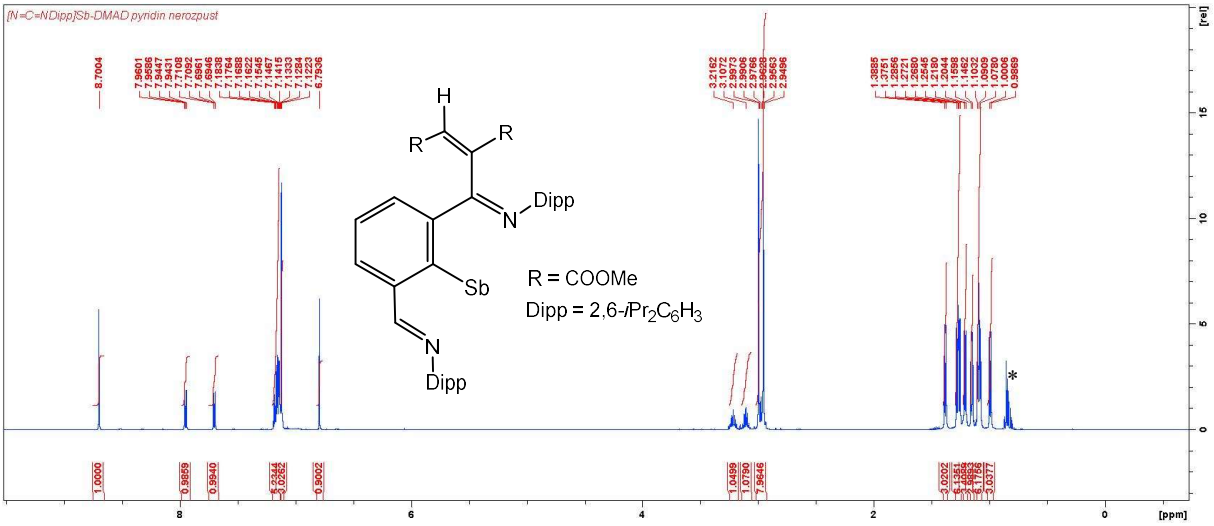


Figure S9: ^{1}H NMR spectrum of **4-Sb** in C_6D_6 (500 MHz). *denotes traces of hexane solvent.

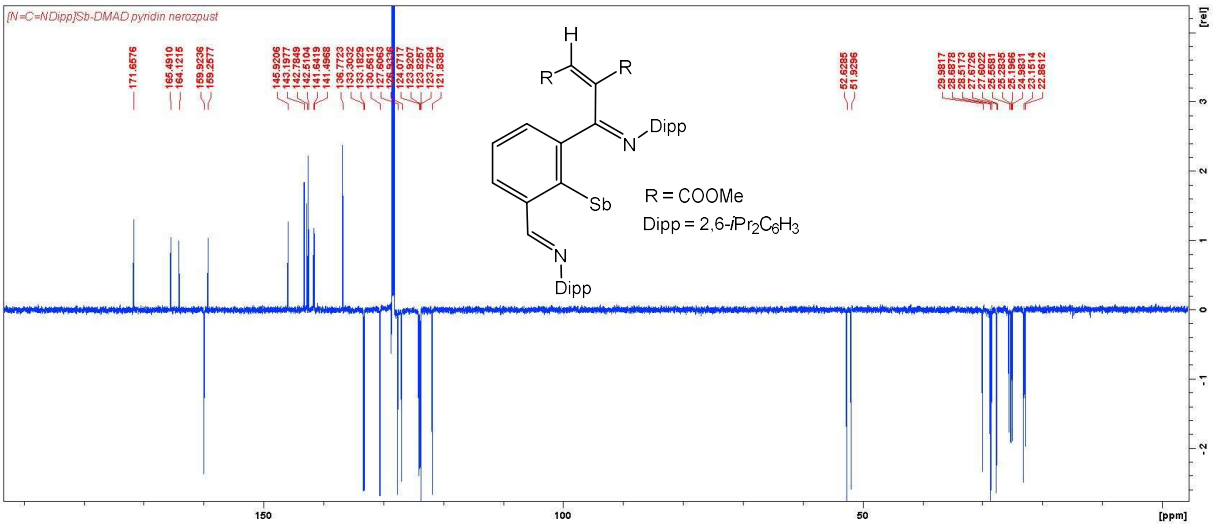


Figure S10: ^{13}C{^{1}H} NMR spectrum of **4-Sb** in C_6D_6 (125.6 MHz).

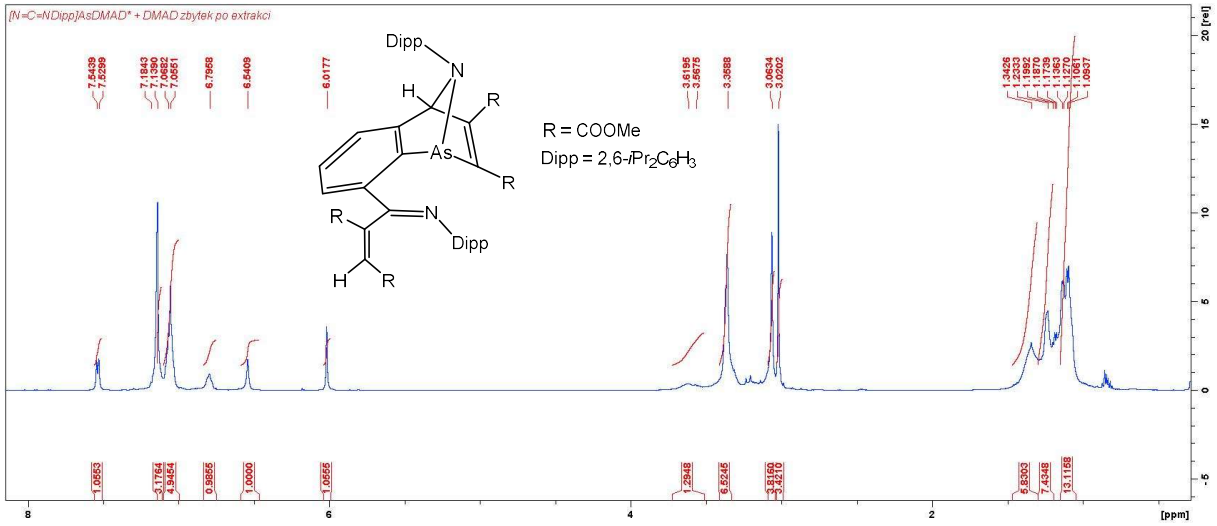


Figure S11: ^{1}H NMR spectrum of **5-As** in C_6D_6 (500 MHz).

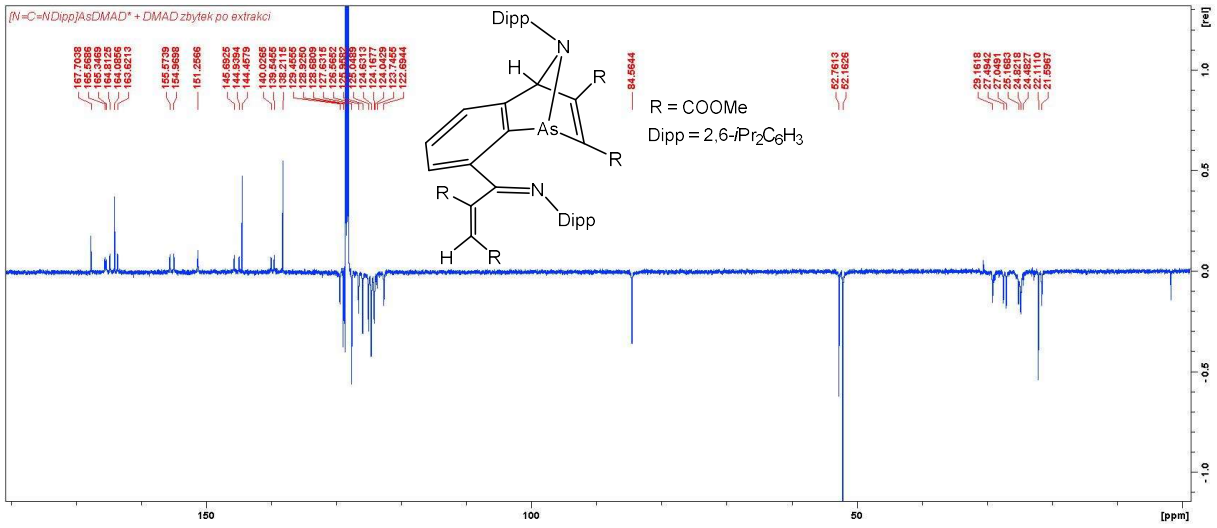


Figure S12: $^{13}C\{^{1}H\}$ NMR spectrum of **5-As** in C_6D_6 (125.6 MHz).

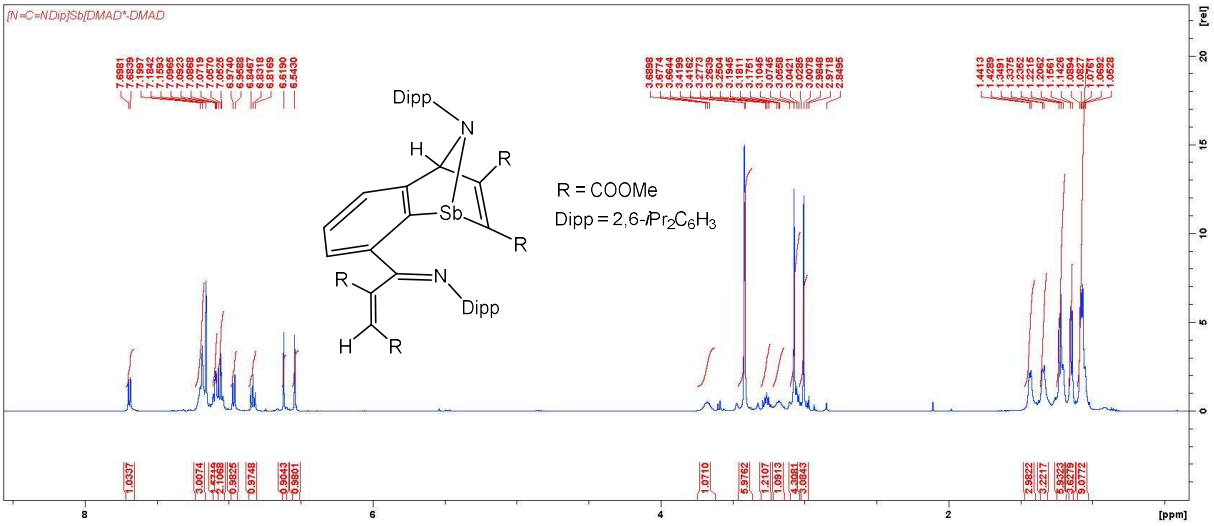


Figure S13: ^{1}H NMR spectrum of **5-Sb** in C_6D_6 (500 MHz).

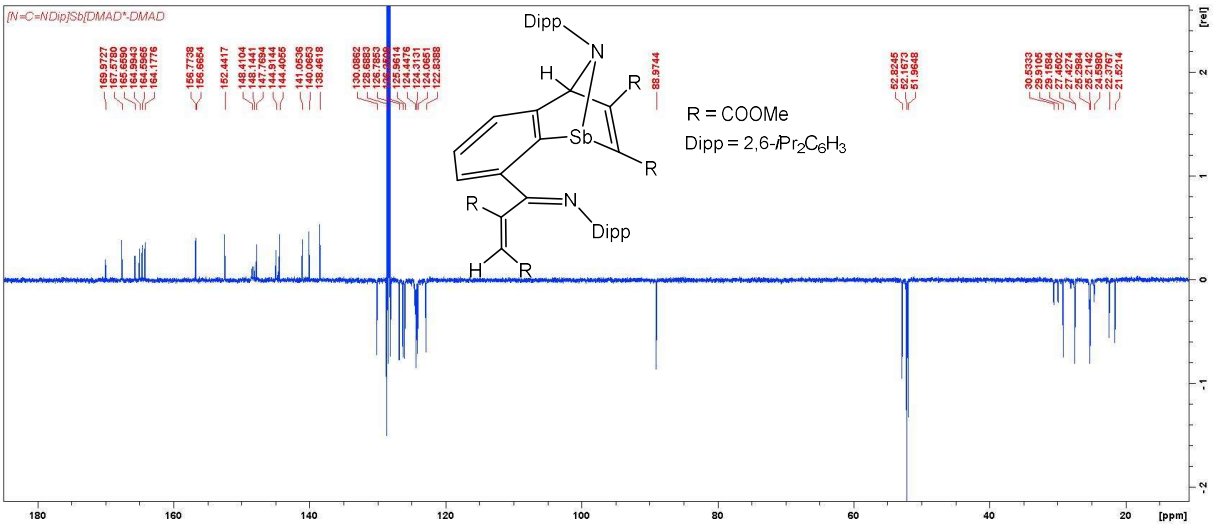


Figure S14: ^{1}H NMR spectrum of **5-Sb** in C_6D_6 (500 MHz).

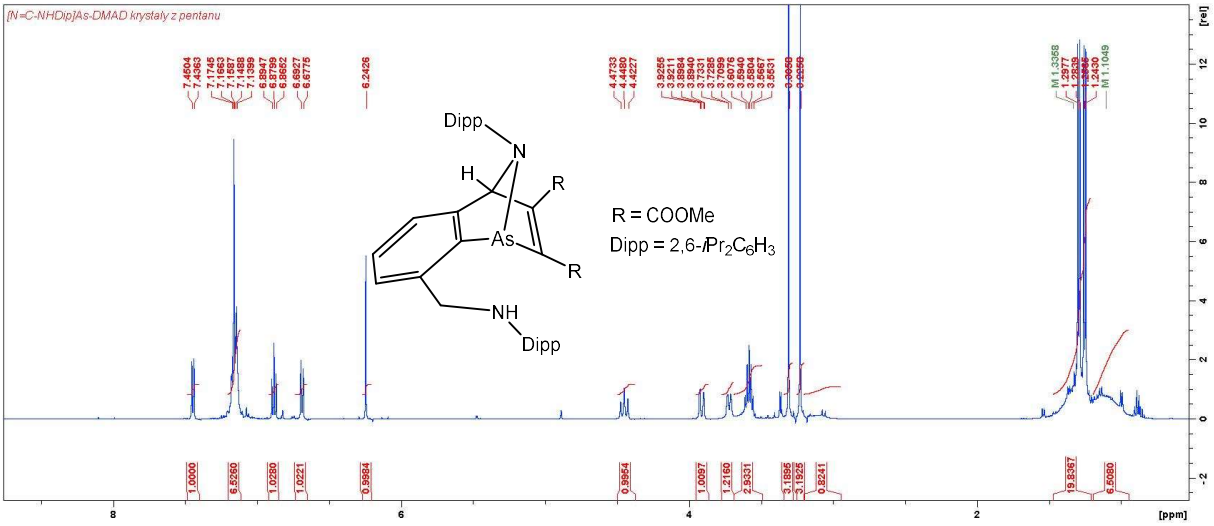


Figure S15: ^{1}H NMR spectrum of **7-As** in C_6D_6 (500 MHz).

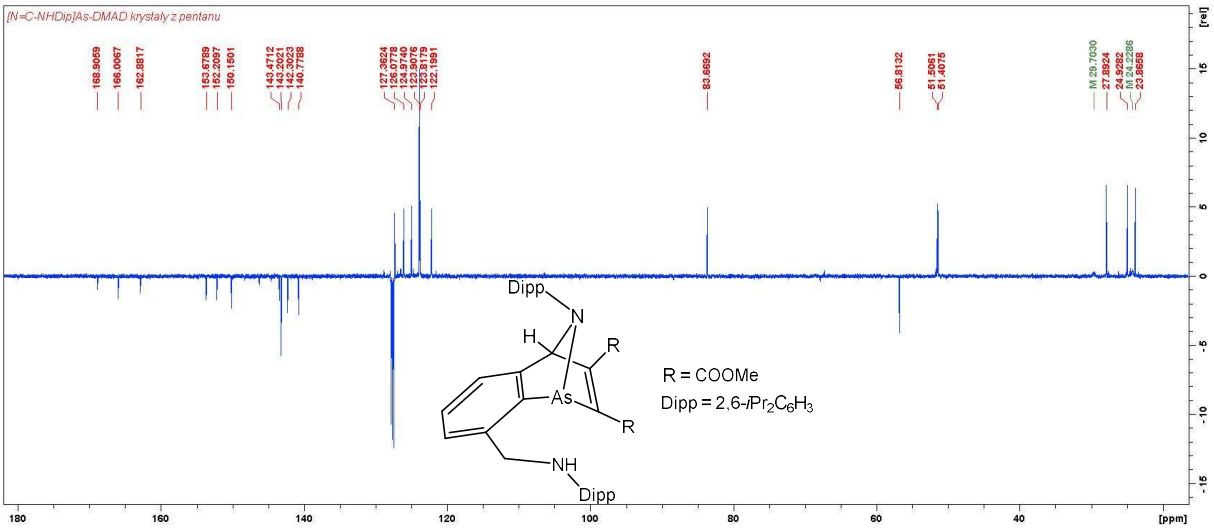


Figure S16: $^{13}C\{^{1}H\}$ NMR spectrum of **7-As** in C_6D_6 (125.6 MHz).

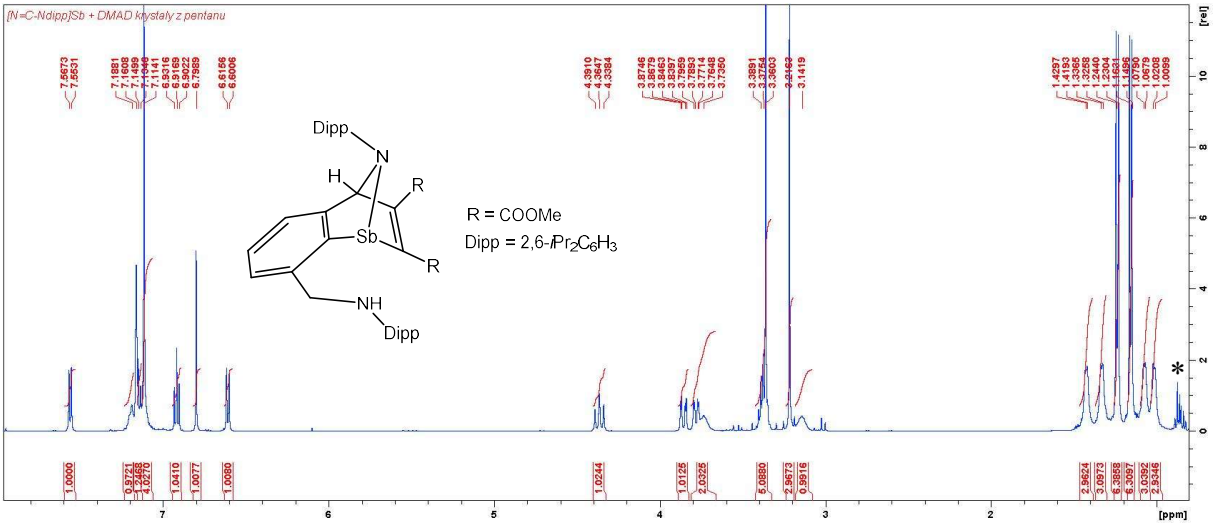


Figure S17: ^{1}H NMR spectrum of **7-Sb** in C_6D_6 (500 MHz). *denotes traces of hexane solvent.

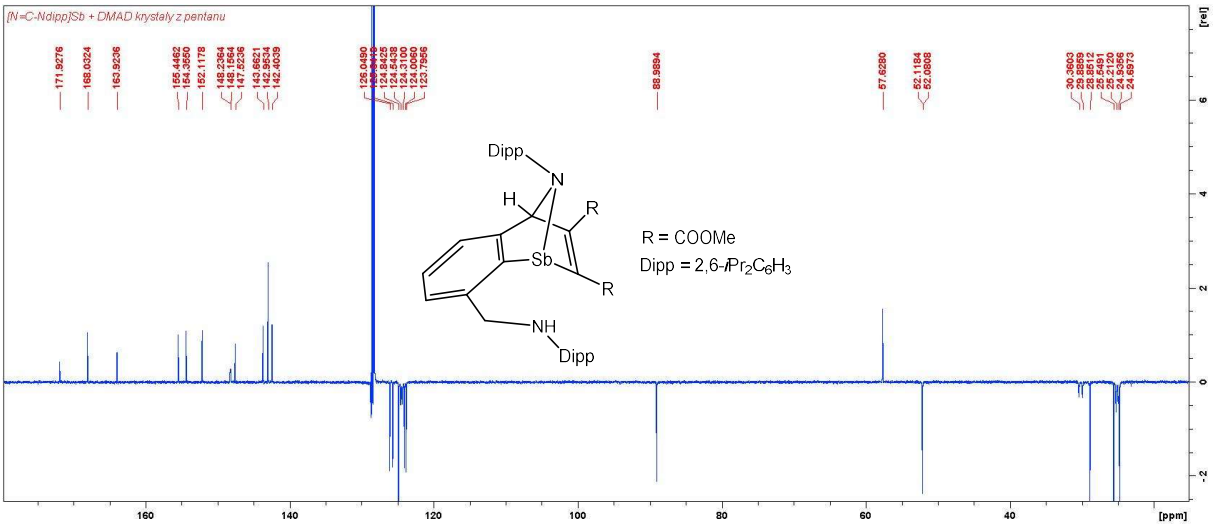


Figure S18: ^{13}C{^{1}H} NMR spectrum of **7-Sb** in C_6D_6 (125.6 MHz).

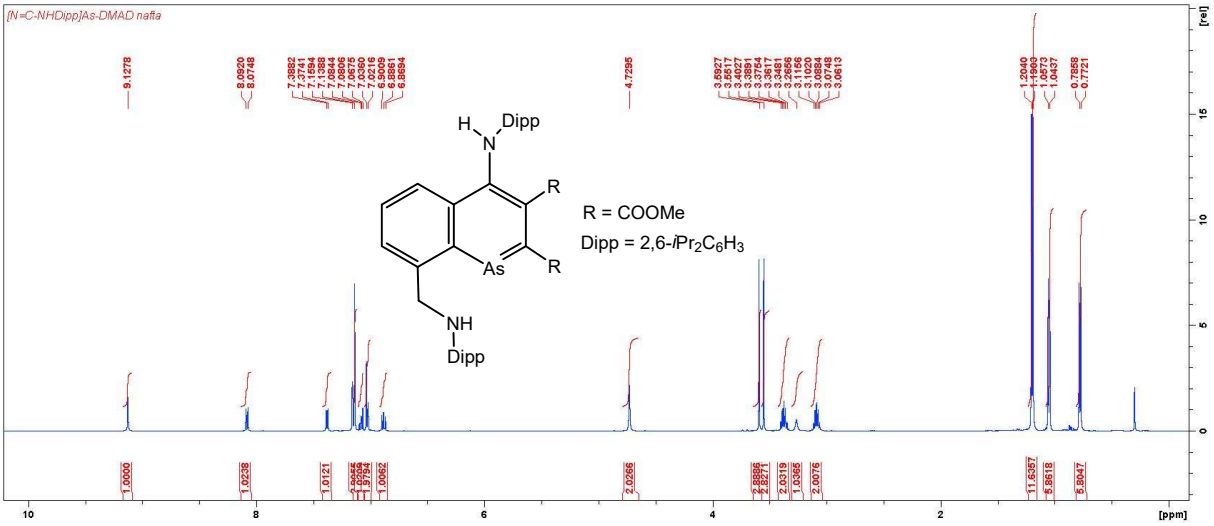


Figure S19: ^{1}H NMR spectrum of **8-As** in C_6D_6 (500 MHz).

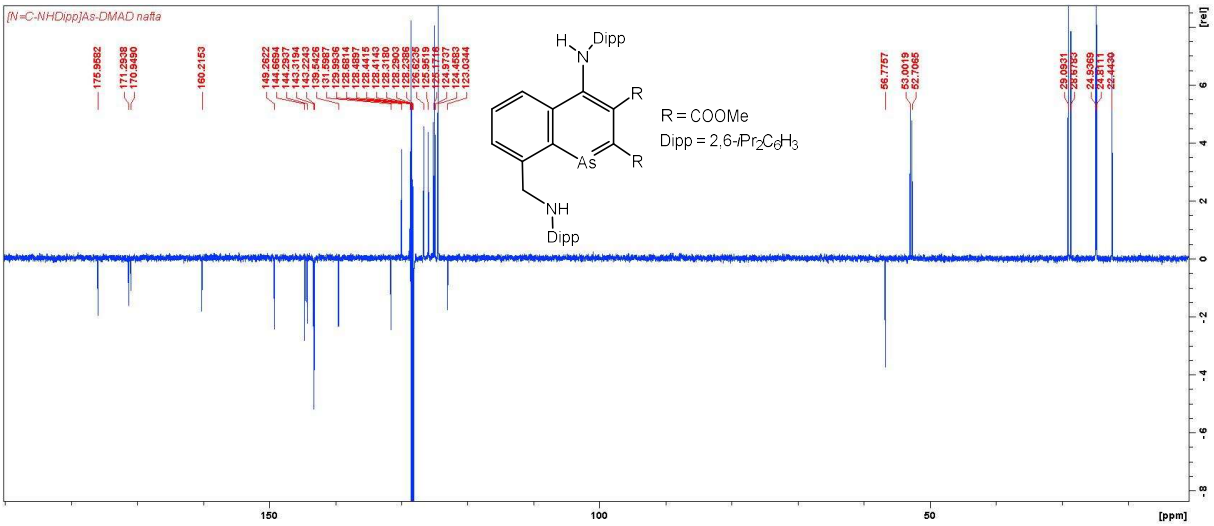


Figure S20: ^{13}C{^{1}H} NMR spectrum of **8-As** in C_6D_6 (125.6 MHz).

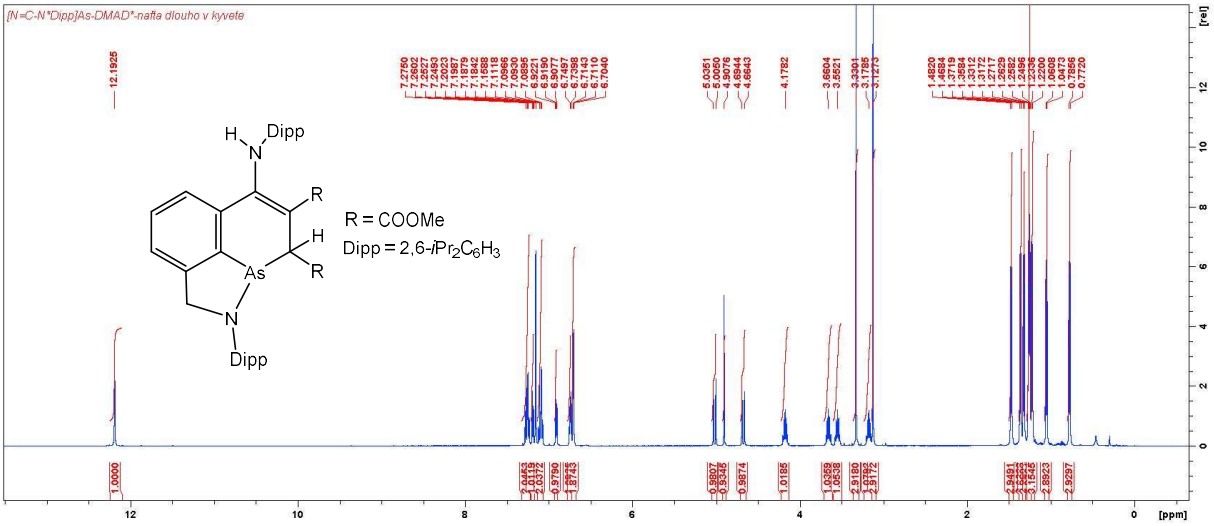


Figure S21: ^{1}H NMR spectrum of **9-As** in C_6D_6 (500 MHz).

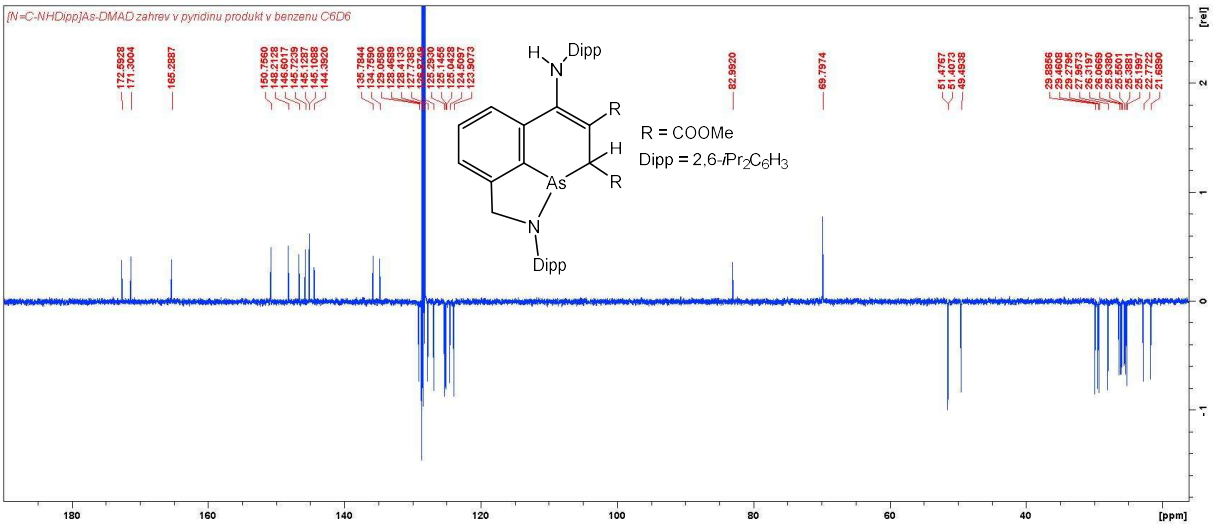


Figure S22: $^{13}C\{^{1}H\}$ NMR spectrum of **9-As** in C_6D_6 (125.6 MHz).

Synthesis 2-Bi

557 mg (0.84 mmol) of **1-Bi** was dissolved in benzene (10 mL) and 104 µL (0.84 mmol) of DMAD was added. The solution was stirred for 1 hour and the original dark green solution turned to brownish. Then it was evaporated and extracted with hexane (20 mL) to give an orange solution that was concentrated to *ca* 1/3 of the original volume. Storage of this mixture at 5 °C provided orange crystals of **2-Bi**, that were collected by decantation and dried in vacuo. Yield 359 mg, 45 %, m.p. 97 °C (dec.). ^{1}H NMR (400 MHz, C_6D_6): δ 0.96 [6H, d(br), *i*Pr-C*H*$_3$]; 1.12

[6H, d, $^{3}J_{H,H}$ = 6.8 Hz, *i*Pr-C*H*$_3$]; 1.17 [6H, d, $^{3}J_{H,H}$ = 6.8 Hz, *i*Pr-C*H*$_3$]; 1.30 [3H, m, *i*Pr-C*H*$_3$]; 1.43 [3H, d(br), *i*Pr-C*H*$_3$]; 2.87 [1H, m(br), *i*Pr-C*H*]; 2.95 [2H, h, $^{3}J_{H,H}$ = 6.8 Hz, *i*Pr-C*H*]; 3.29 [3H, s, OC*H*$_3$]; 3.51 [3H, s, OC*H*$_3$]; 3.75 [1H, m(br), *i*Pr-C*H*]; 6.86 [1H, d, $^{3}J_{H,H}$ = 7.3 Hz, Ar-*H*]; 6.97 [1H, t, $^{3}J_{H,H}$ = 7.3 Hz, Ar-*H*]; 7.12 [1H, m(br), Ar-*H*]; 7.16 [5H, m, Ar-*H*]; 8.05 [1H, s, C*H*=N]; 8.10 [1H, d, $^{3}J_{H,H}$ = 7.3 Hz, Ar-*H*]; 9.35 [1H, s, C*H*]. $^{13}C\{^{1}H\}$ NMR (125.76 MHz, C_6D_6): δ 24.0 [*i*Pr-C*H*$_3$]; 24.1 [*i*Pr-C*H*$_3$]; 25.0 [*i*Pr-C*H*$_3$]; 25.1 [*i*Pr-C*H*$_3$]; 29.0 [*i*Pr-C*H*]; 29.8 [*i*Pr-C*H*]; 51.9 [O*C*H$_3$]; 52.2 [O*C*H$_3$]; 105.8 [*C*H]; 123.8 [Ar-*C*]; 125.5 [Ar-*C*]; 125.6 [Ar-*C*]; 128.2 [Ar-*C*]; 128.9 [Ar-*C*]; 129.0 [Ar-*C*]; 138.4 [Ar-*C*]; 141.1 [Ar-*C*]; 149.1 [Ar-*C*]; 151.0 [Ar-*C*]; 155.1 [*C*=*C*]; 157.7 [Ar-*C*] ; 165.2 [*C*H=N]; 167.1 [*C*=O]; 173.6 [*C*=O]; 189.4 [Ar-*C*]; 191.2 [*C*=*C*] ppm.

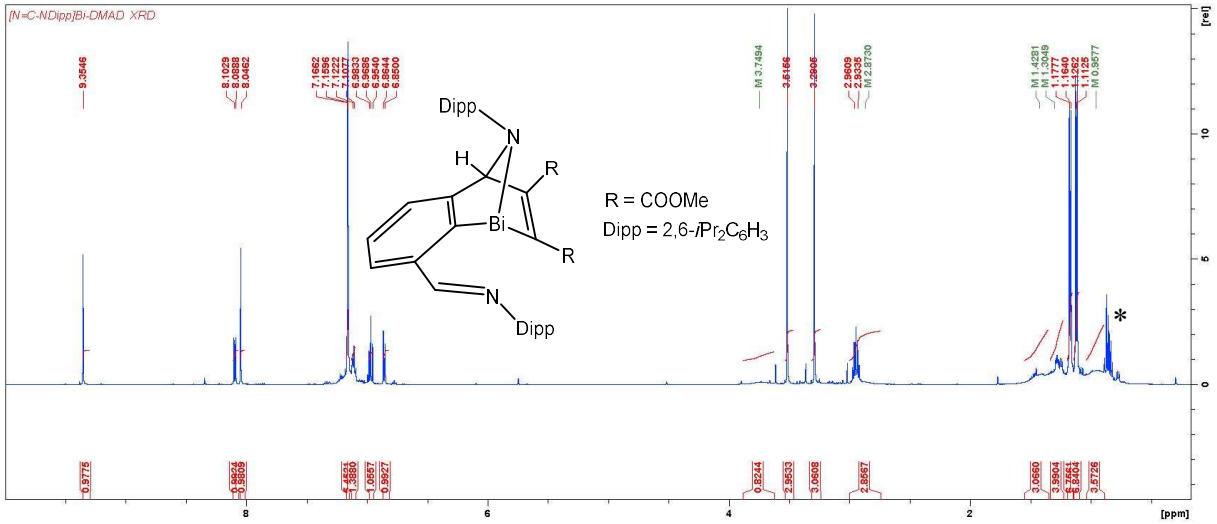


Figure S23: ^{1}H NMR spectrum of **2-Bi** in C_6D_6 (500 MHz). *denotes traces of hexane solvent.

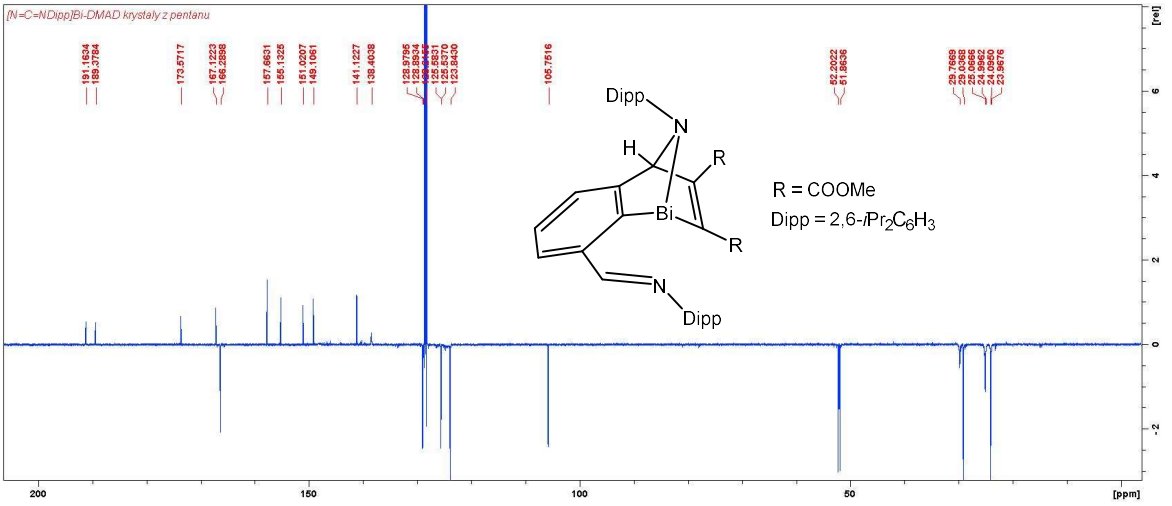


Figure S24: $^{13}C\{^{1}H\}$ NMR spectrum of **2-Bi** in C_6D_6 (125.6 MHz).

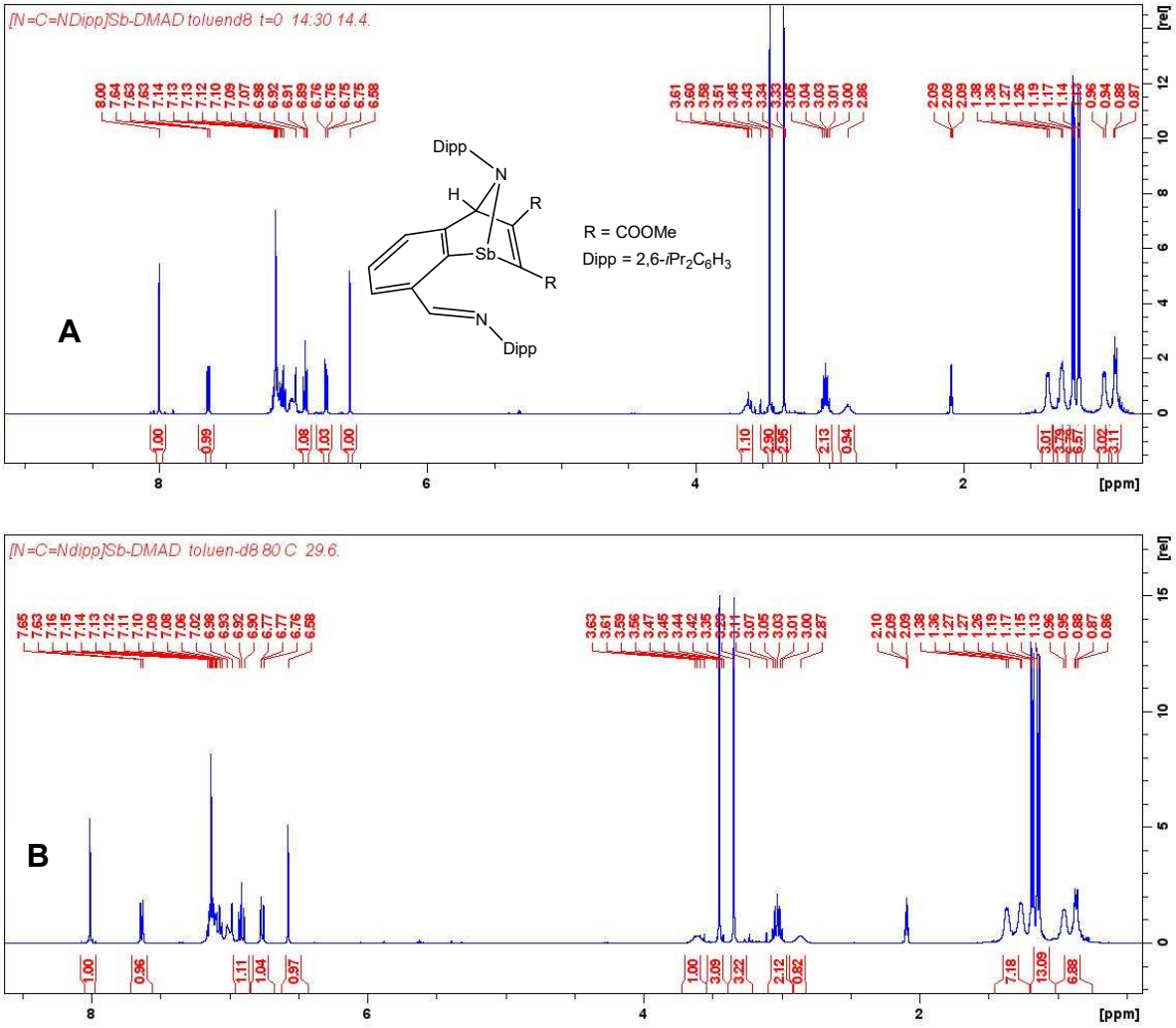


Figure S25: ^{1}H NMR spectra showing heating of **2-Sb** in C_6D_6 to 80 °C in a sealed NMR tube at the start (**A**, 500 MHz) and after more than 2 months (**B**, 400 MHz).

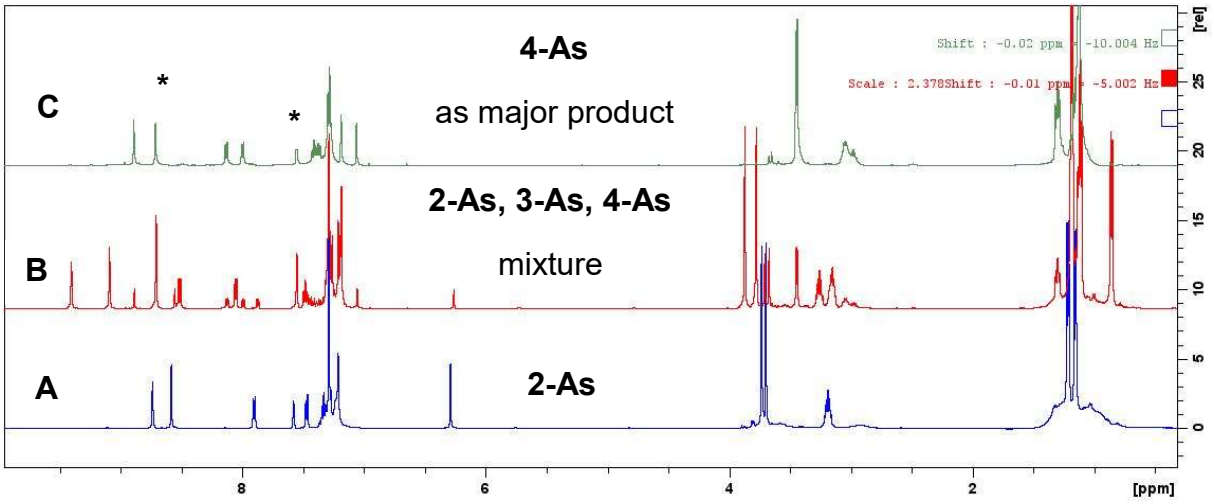


Figure S26: ^{1}H NMR spectra showing heating of **2-As** in pyridine-d_5 to 65 °C in a sealed NMR tube (500 MHz), **A** t=0, **B** t = 3h, **C** t = 24 h. *denotes residual signals of pyridine-d_5.

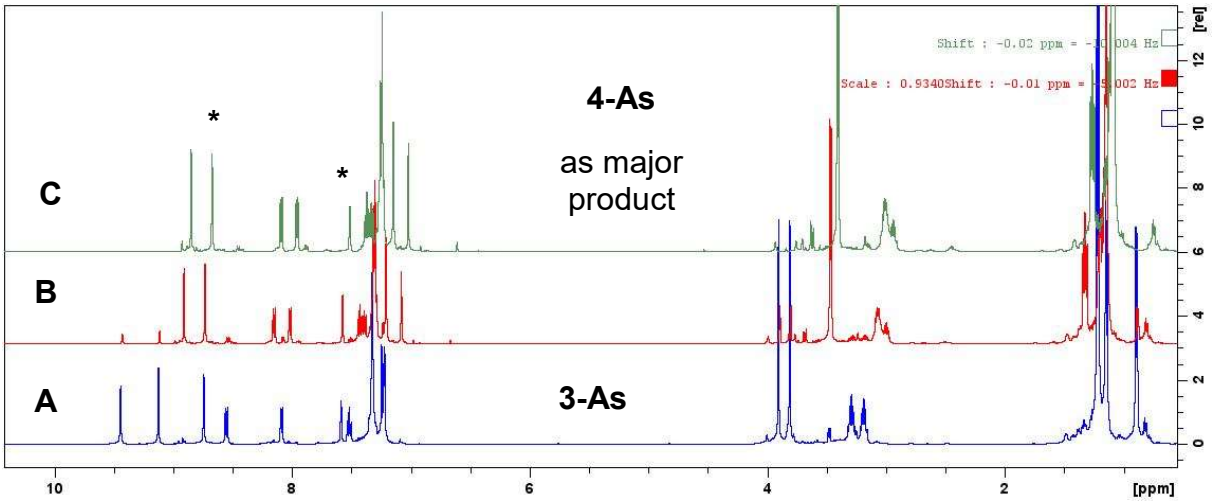


Figure S27: ^{1}H NMR spectra showing heating of **3-As** in pyridine-d_5 to 65 °C in a sealed NMR tube (500 MHz), **A** t=0, **B** t = 3h, **C** t = 24 h. *denotes residual signals of pyridine-d_5.

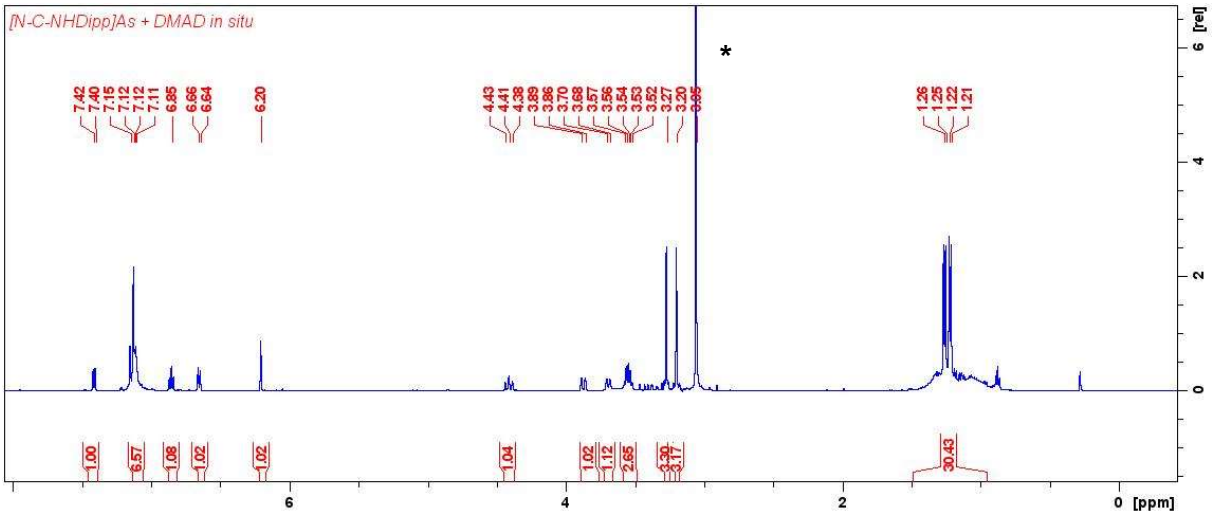


Figure S28: ^{1}H NMR spectrum showing the reaction mixture after addition of an excess of DMAD (*) toward **6-As** in C_6D_6 in an NMR tube (500 MHz) showing almost clean formation of **7-As** as the product.

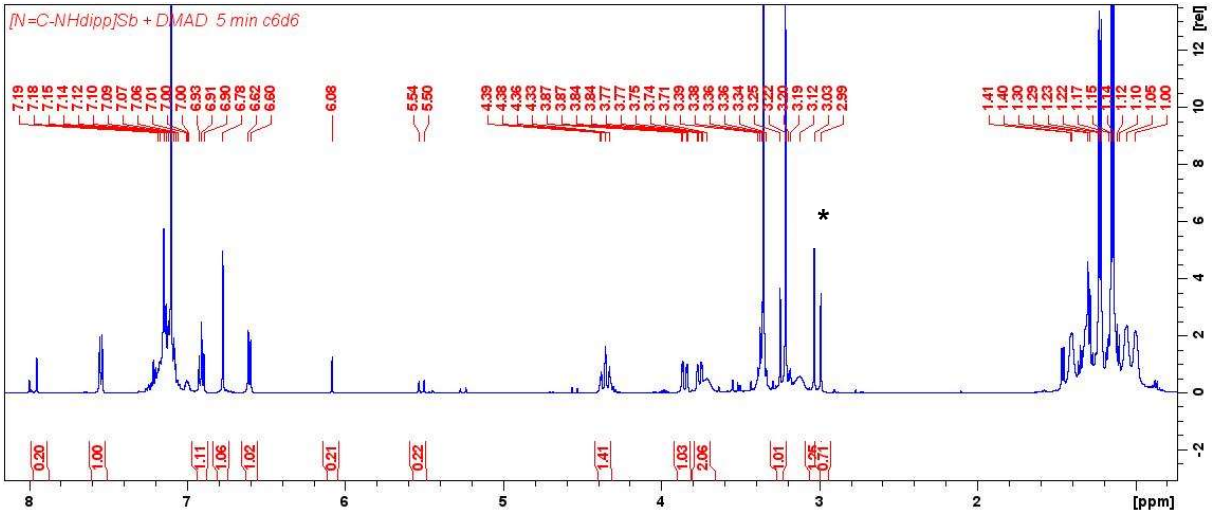


Figure S29: ^{1}H NMR spectrum showing the reaction mixture after addition of an excess of DMAD (*) toward **6-Sb** in C_6D_6 in an NMR tube (500 MHz) showing mixture of products **7-Sb** being the main component.

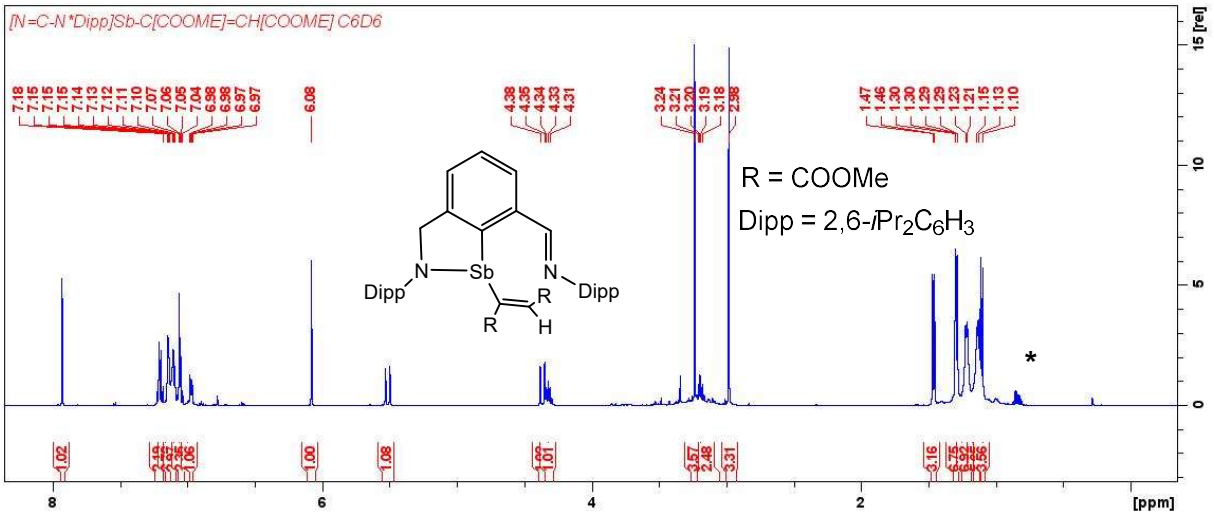


Figure S30: ^{1}H NMR spectrum of **10-Sb** in C_6D_6 (500 MHz). *denotes traces of hexane solvent.

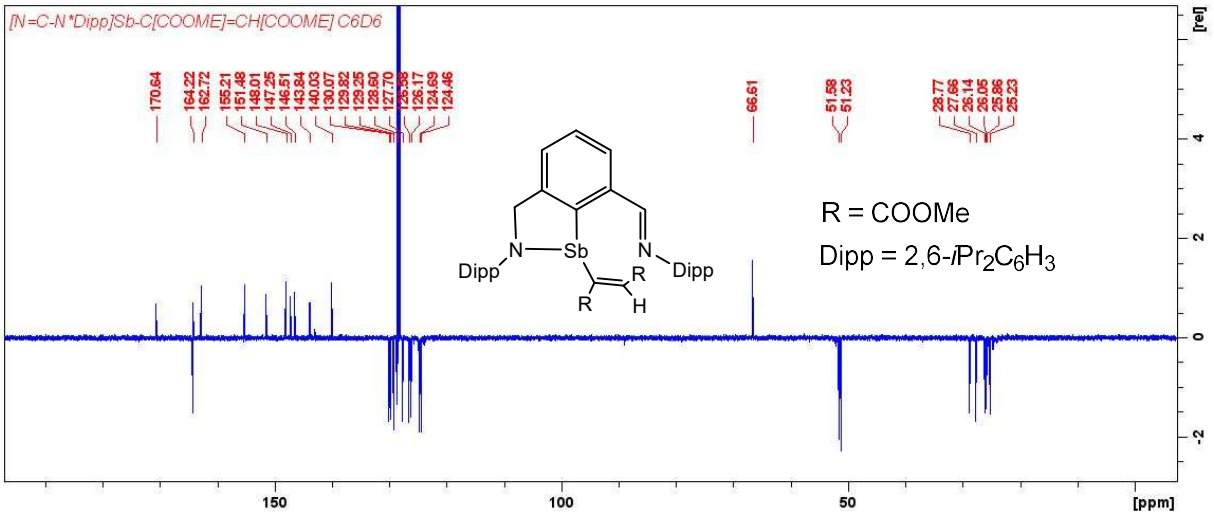


Figure S31: ^{13}C{^{1}H} NMR spectrum of **10-Sb** in C_6D_6 (125.6 MHz).

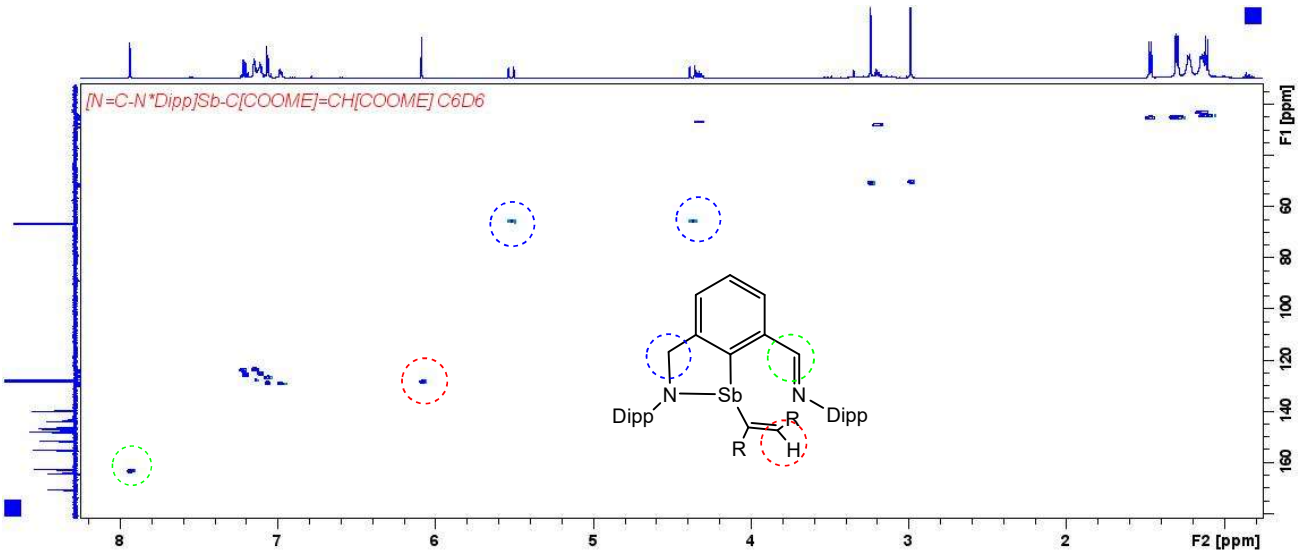


Figure S32: HSQC NMR spectrum of **10-Sb** in C_6D_6

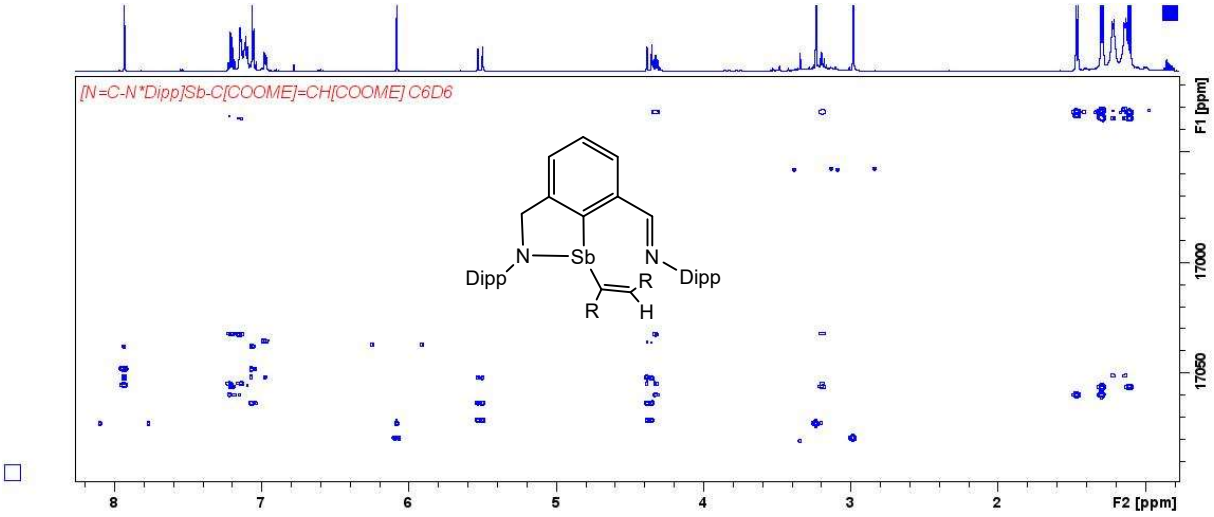


Figure S33: HMBC NMR spectrum of **10-Sb** in C_6D_6.

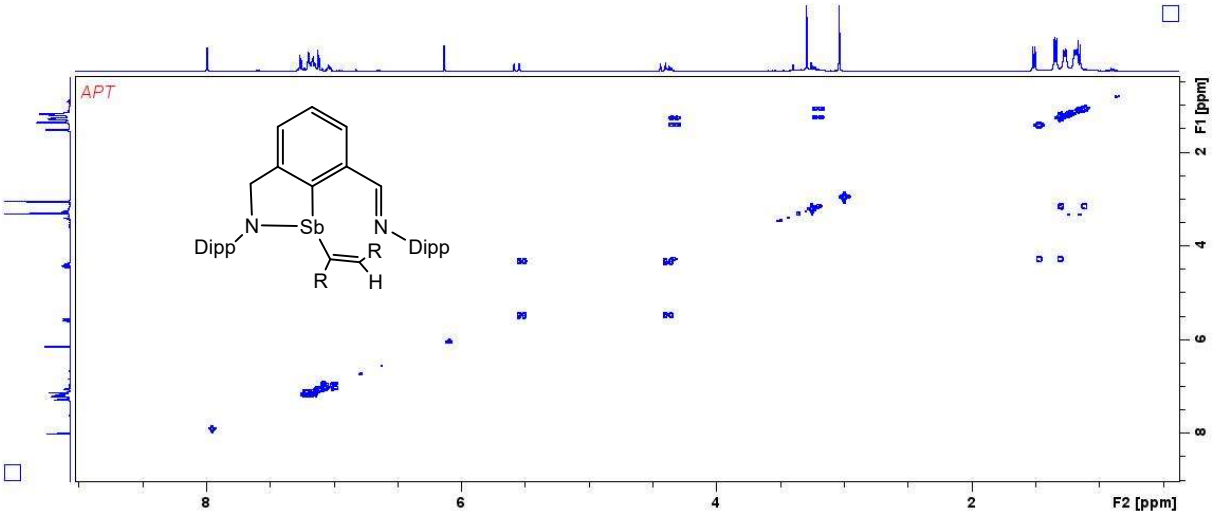


Figure S34: H,H COSY NMR spectrum of **10-Sb** in C_6D_6 (400 MHz).

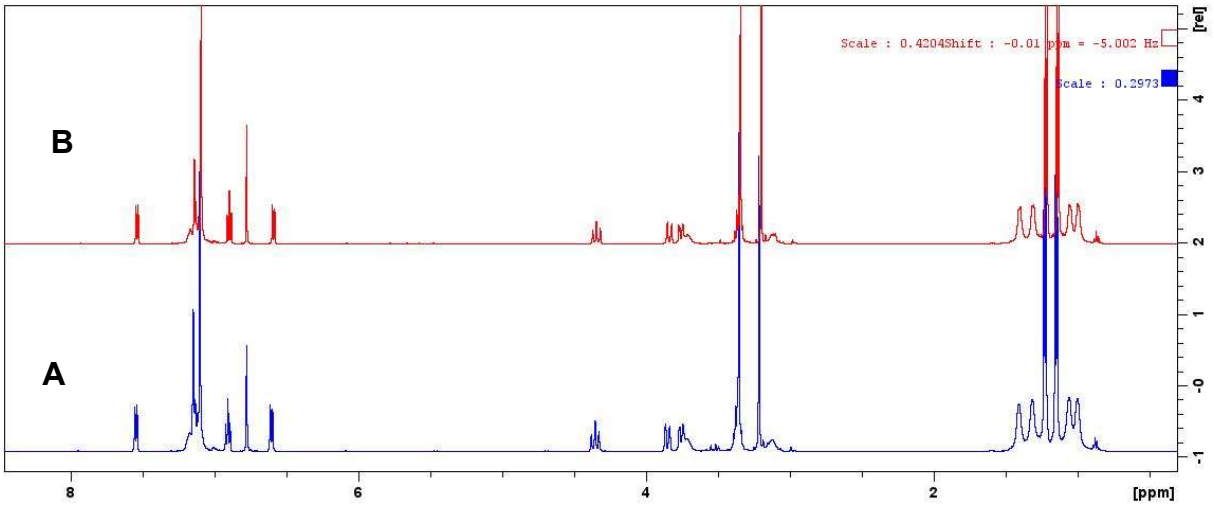


Figure S35: ^{1}H NMR spectra demonstrating the stability of **7-Sb** in C_6D_6 at ambient temperature (500 MHz), **A** t=0, **B** t = 14 days.

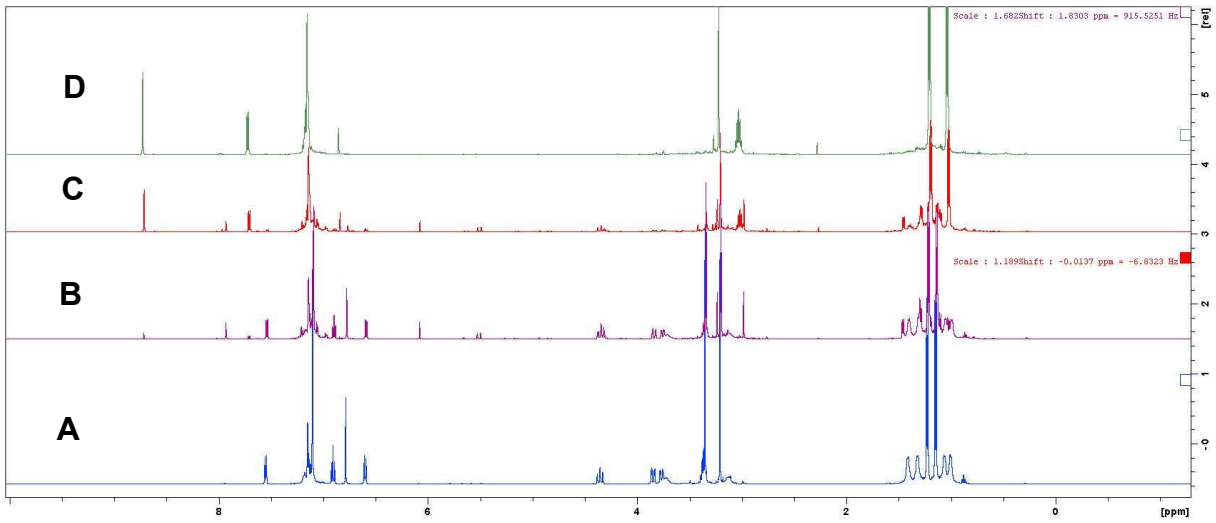


Figure S36: ^{1}H NMR spectra demonstrating heating of **7-Sb** sealed in C_6D_6 to 80°C (500 MHz). **A** t=0, **B** t = 1 month, **C** t = 2 months, **D** t = 3 months.

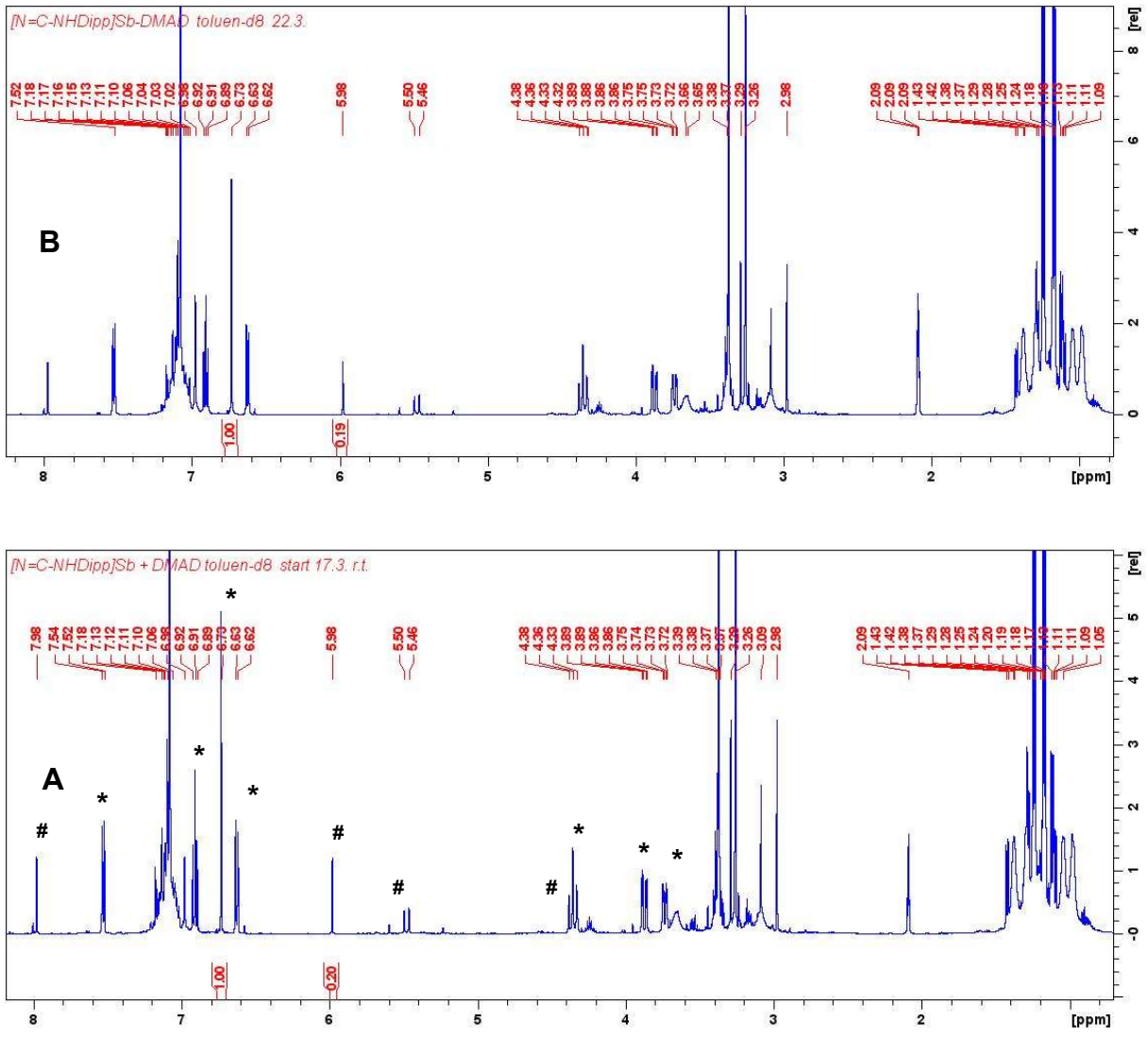


Figure S37: ^{1}H NMR spectra of crude reaction mixture of **6-Sb** and DMAD in toluene-d_8 (500 MHz) containing products **7-Sb** (*) and **10-Sb** (#)**, A** t=5 min, **B** t = 5 days.

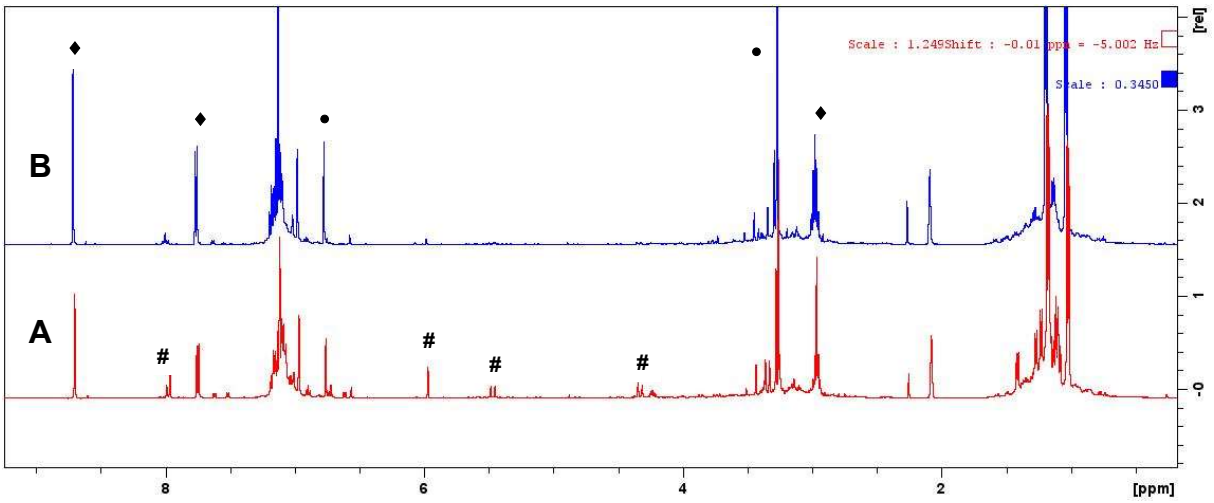


Figure S38: ^{1}H NMR spectra of mixture of **6-Sb** and DMAD in toluene-d8 (500 MHz) containing **10-Sb** (#) heated to 100 °C producing **1-Sb** (♦) along with dimethylfumarate (•). **A** t=24 hod, **B** t = 5 days.

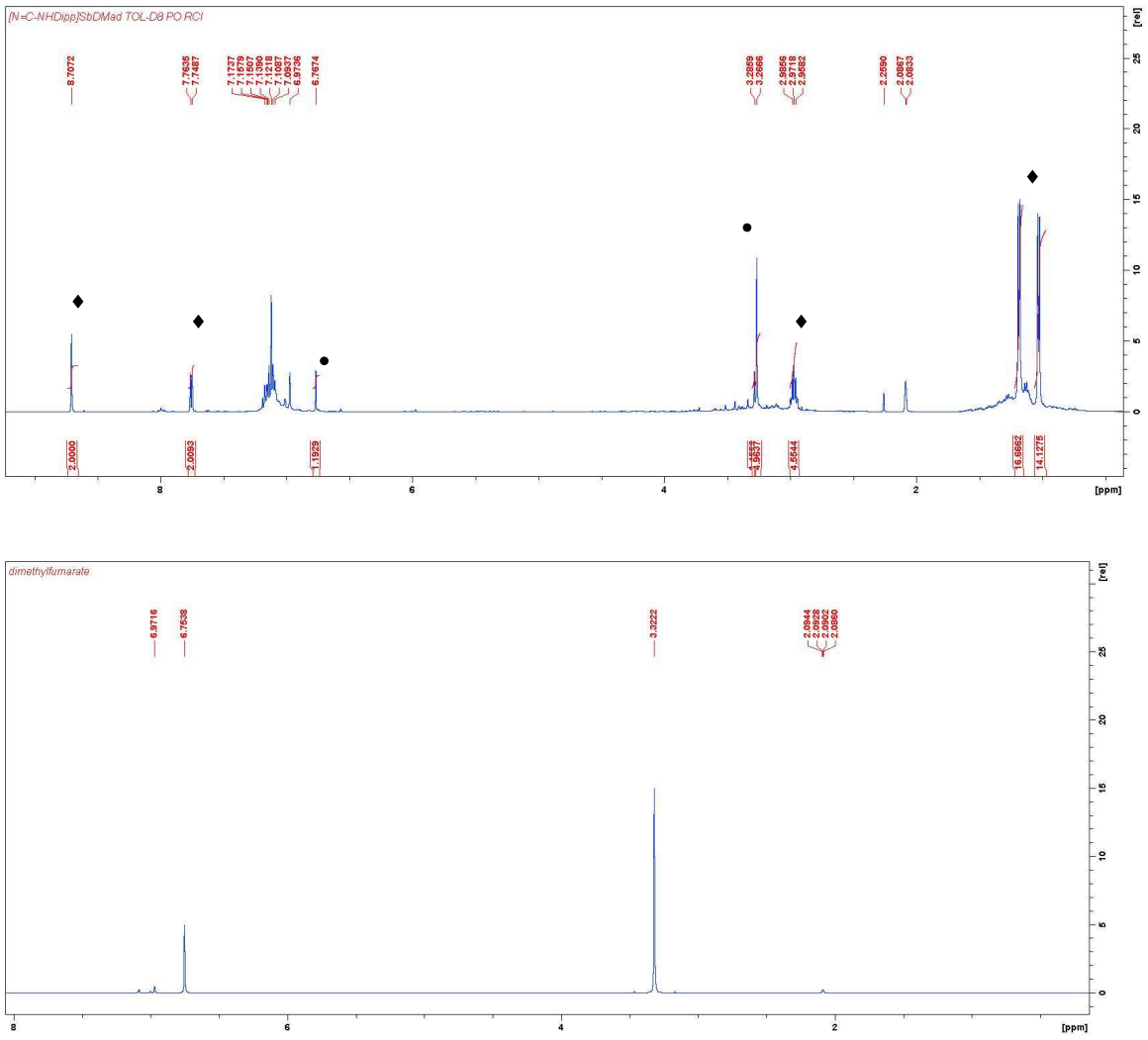


Figure S39: Comparison of ^{1}H NMR spectra of mixture of **1-Sb** (♦) along with dimethylfumarate (●) vs. pure dimethylfumarate (lower spectrum) obtained after reaction with pure alkenes toluene-d_8 (500 MHz).

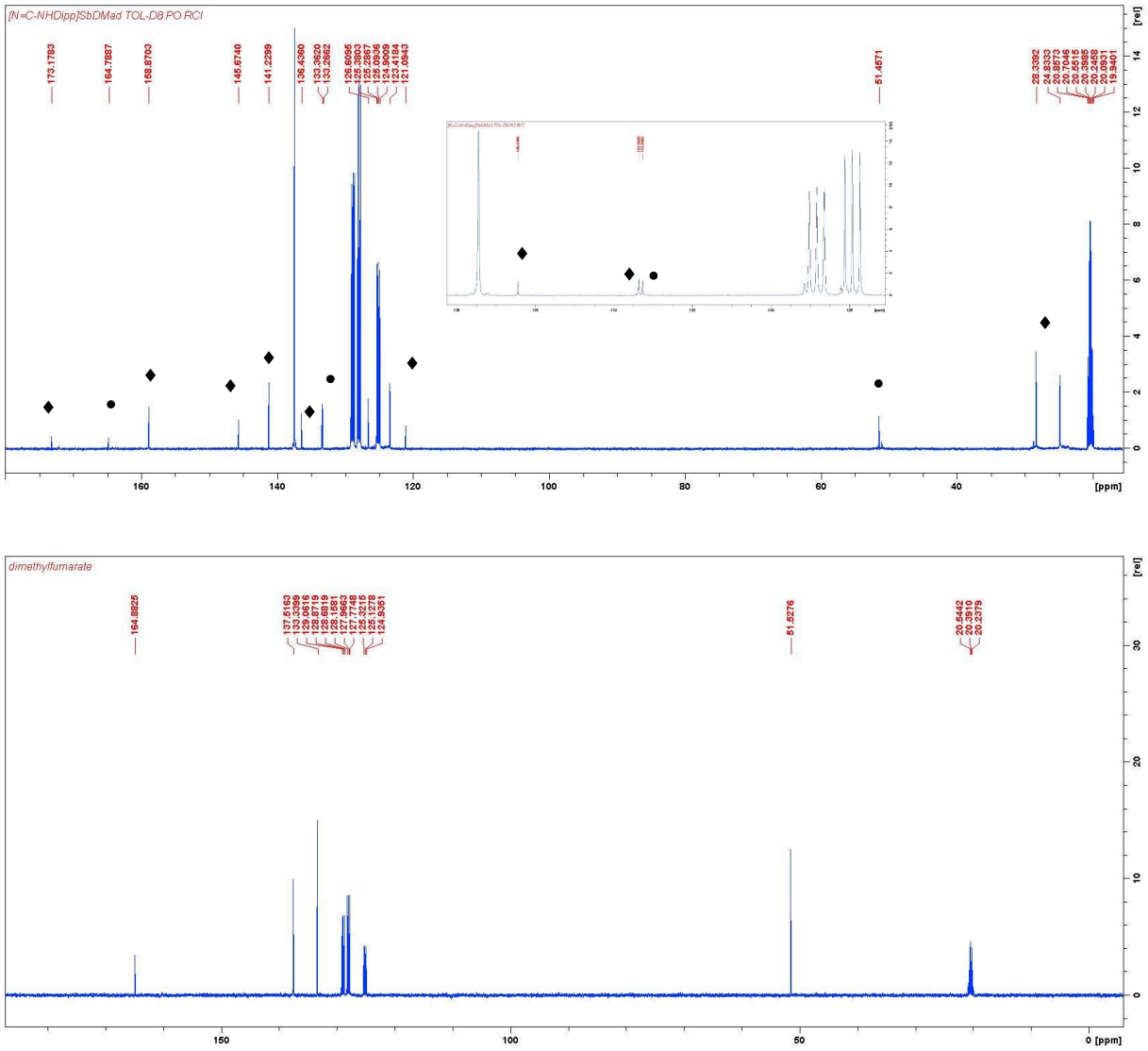


Figure S40: Comparison of ^{13}C NMR spectra of mixture of **1-Sb** (♦) along with dimethylfumarate (●) vs. pure dimethylfumarate (lower spectrum) obtained after reaction with pure alkenes toluene-d_8 (125.6 MHz).

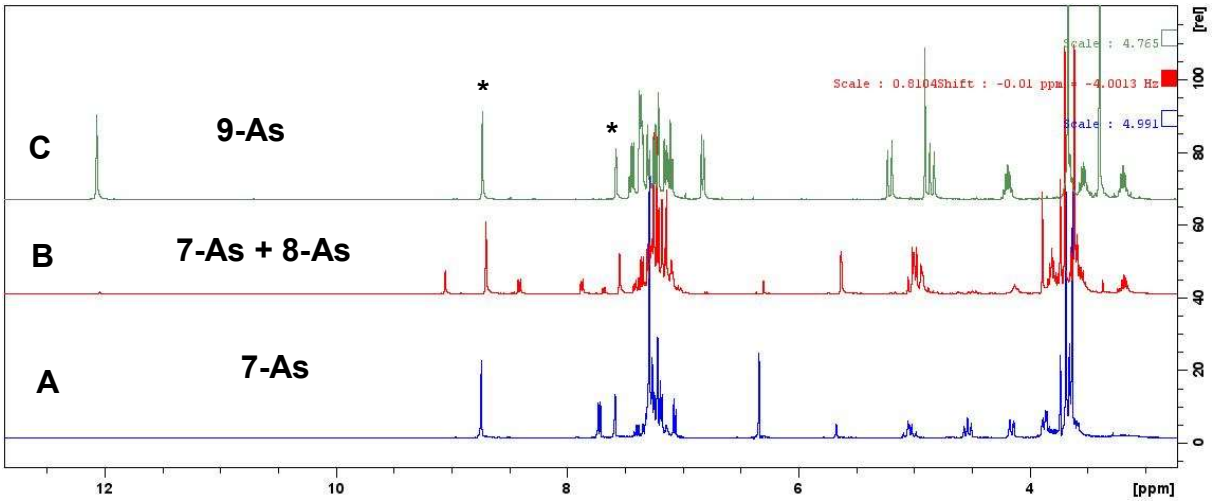


Figure S41: ^{1}H NMR spectra showing heating of **7-As** in pyridine-d_5 to 65 °C in a sealed NMR tube (400 MHz), **A** t=0, **B** t = 1h, **C** t = 12 h. *denotes residual signals of pyridine-d_5.

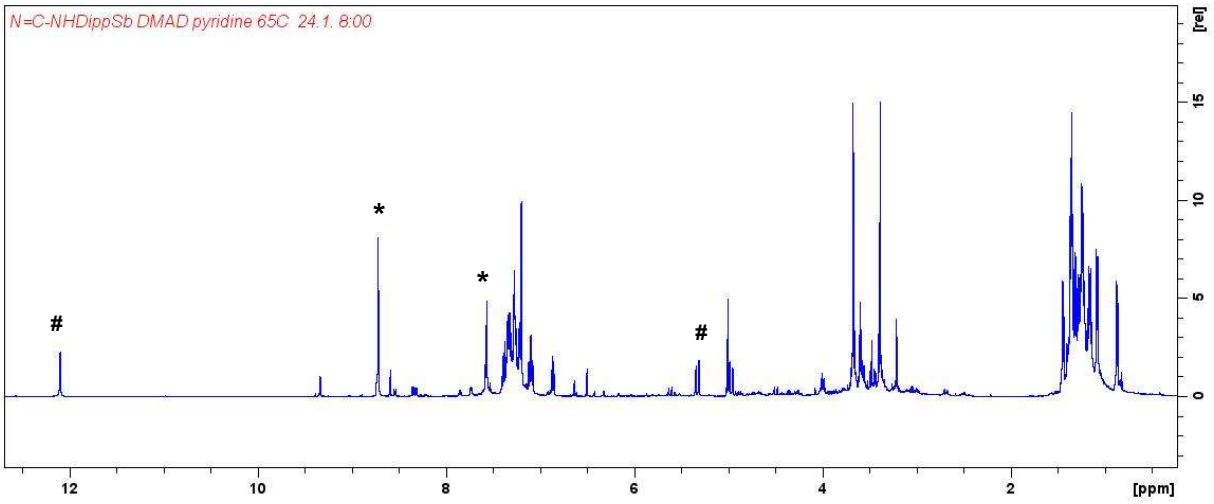


Figure S42: ^{1}H NMR spectra of mixture obtained after heating of **7-Sb** in pyridine-d_5 to 65 °C for 5 days suggesting the presence of the intended product **9-Sb** (#) (500 MHz). *denotes residual signals of pyridine-d_5.

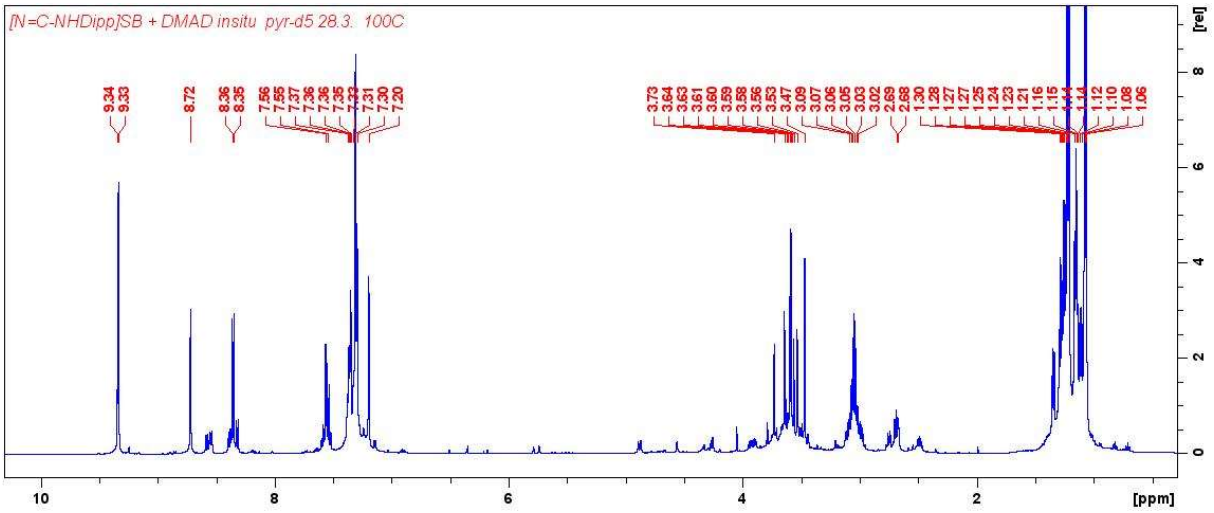


Figure S43: ^{1}H NMR spectra of mixture of **6-Sb** and DMAD in pyridine-d_5 (500 MHz) heated to 80 °C for 5 days.

2. Crystallographic data.

Table S1. Crystal data and structure refinement of studied compounds.

	2-As	**2-Sb**	**2-Bi**
Formula	$C_{38}H_{45}AsN_2O_4$	$C_{38}H_{45}N_2O_4Sb$	$C_{38}H_{45}BiN_2O_4$
Formula weight, g mol^{-1}	668.68	715.51	802.74
Crystal system	Triclinic	Triclinic	Orthorhombic
Crystal size, mm	0.52 × 0.32 × 0.23	0.59 × 0.35 × 0.10	0.36 × 0.11 × 0.07
Space group	P-1	P-1	$Pna2_1$
a, Å	10.2024(7)	10.0390(4)	22.8568(7)
b, Å	11.4261(7)	11.2202(4)	10.9255(4)
c, Å	16.6186(10)	17.4320(6)	28.4085(8)
α, º	102.369(3)	102.590(2)	90
β, º	99.956(3)	97.846(2)	90
γ, º	107.749(3)	107.829(2)	90
V, Å^3	1742.2(2)	1780.10(12)	7094.2(4)
Z	2	2	8
ρ_{calcd}, Mg m^{-3}	1.275	1.335	1.503
μ (Mo $K\alpha$), mm^{-1}	1.016	0.815	5.011
F(000)	704	740	3216
θ range, deg	1 to 27.5	1 to 27.5	1 to 27.5
No. of reflns collected	51025	57227	65003
No. indep. Reflns	8056	8216	16139
No. obsd reflns with ($I>2\sigma(I)$), R_{int}	6873, 0.044	6656, 0.057	10821, 0.15
No. refined params	422	419	827
GooF (F^2)	1.057	1.078	1.005
R_1 (F) ($I > 2\sigma(I)$)	0.063	0.044	0.063
wR_2 (F^2) (all data)	0.113	0.076	0.081
Largest diff peak/hole, e Å^{-3}	1.107 / –0.808	0.554 / –0.868	1.646 / –1.857
CCDC	2192914	2192911	2192912

$R_{int} = \sum |F_o^2 - F_{o,mean}^2| / \sum F_o^2$, $S = [\sum(w(F_o^2 - F_c^2)^2)/(N_{diffrs} - N_{params})]^{½}$ for all data, $R(F) = \sum ||F_o| - |F_c|| / \sum |F_o|$ for observed data, $wR(F^2) = [\sum(w(F_o^2 - F_c^2)^2)/(\sum w(F_o^2)^2)]^{½}$ for all data.

Table S1 (continuation). Crystal data and structure refinement of studied compounds.

	4-Sb	**5-As**	**5-Sb**
Formula	$C_{38}H_{45}N_2O_4Sb.(C_6H_6)$	$C_{44}H_{51}AsN_2O_8$	$C_{44}H_{51}N_2O_8Sb$
Formula weight, g mol^{-1}	793.61	810.78	857.61
Crystal system	Triclinic	Triclinic	Triclinic
Crystal size, mm	0.59 × 0.26 × 0.07	0.59 × 0.26 × 0.06	0.59 × 0.46 × 0.30
Space group	P-1	P-1	P-1
a, Å	8.7928(3)	11.405(2)	11.361(3)
b, Å	11.5342(4)	14.254(3)	14.190(3)
c, Å	20.5702(7)	14.960(3)	15.078(3)
α, º	76.875(2)	72.640(8)	89.581(8)
β, º	87.983(3)	70.438(9)	71.665(9)
γ, º	77.437(2)	68.085(9)	66.480(9)
V, Å^3	1982.82(12)	2083.3(7)	2096.1(8)
Z	2	2	2
ρ_{calcd}, Mg m^{-3}	1.329	1.292	1.359
μ (Mo $K\alpha$), mm^{-1}	0.739	0.869	0.712
F(000)	824	852	888
θ range, deg	1 to 27.5	1 to 27.5	1 to 27.5
No. of reflns collected	69042	31555	41762
No. indep. Reflns	9170	7492	10322
No. obsd reflns with ($I>2\sigma(I)$), R_{int}	8107, 0.032	6079, 0.082	9170, 0.036
No. refined params	458	517	508
GooF (F^2)	1.085	1.095	1.000
R_1 (F) ($I > 2\sigma(I)$)	0.032	0.061	0.028
wR_2 (F^2) (all data)	0.067	0.158	0.064
Largest diff peak/hole, e Å^{-3}	0.603 / –0.565	0.822 / –1.333	0.611 / –0.818
CCDC	2192913	2192918	2192916

$R_{int} = \sum |F_o^2 - F_{o,mean}^2| / \sum F_o^2$, $S = [\sum(w(F_o^2 - F_c^2)^2)/(N_{diffrs} - N_{params})]^{½}$ for all data, $R(F) = \sum ||F_o| - |F_c|| / \sum |F_o|$ for observed data, $wR(F^2) = [\sum(w(F_o^2 - F_c^2)^2)/(\sum w(F_o^2)^2)]^{½}$ for all data.

Table S1 (continuation). Crystal data and structure refinement of studied compounds.

	7-Sb	**8-As**	**9-As**
Formula	$C_{38}H_{47}N_2O_4Sb$	$C_{38}H_{47}AsN_2O_4$	$C_{38}H_{47}AsN_2O_4$
Formula weight, g mol^{-1}	717.52	670.69	670.69
Crystal system	Triclinic	Triclinic	Monoclinic
Crystal size, mm	0.33 × 0.26 × 0.22	0.43 × 0.30 × 0.16	0.29 × 0.24 × 0.08
Space group	P-1	P-1	C2/c
a, Å	9.8206(4)	11.1958(5)	30.1953(13)
b, Å	10.0140(4)	12.5602(6)	10.8768(5)
c, Å	19.2579(6)	12.8491(6)	25.0422(16)
α, º	91.373(2)	89.006(2)	90
β, º	103.932(2)	80.027(2)	123.4430(10)
γ, º	104.657(2)	80.477(2)	90
V, Å^3	1780.27(12)	1759.59(14)	6862.9(6)
Z	2	2	8
ρ_{calcd}, Mg m^{-3}	1.339	1.266	1.298
μ (Mo $K\alpha$), mm^{-1}	0.815	1.007	1.032
F(000)	744	708	2832
θ range, deg	1 to 27.5	1 to 27.5	1 to 27.5
No. of reflns collected	61486	54993	89196
No. indep. Reflns	8209	8124	7910
No. obsd reflns with ($I>2\sigma(I)$), R_{int}	7414, 0.033	6961, 0.035	6206, 0.043
No. refined params	420	424	420
GooF (F^2)	1.085	1.045	1.028
R_1 (F) ($I > 2\sigma(I)$)	0.033	0.034	0.041
wR_2 (F^2) (all data)	0.075	0.075	0.078
Largest diff peak/hole, e Å^{-3}	1.171 / –0.839	0.549 / –0.463	0.716 / –0.598
CCDC	2192915	2192919	2192917

$R_{int} = \sum |F_o^2 - F_{o,mean}^2| / \sum F_o^2$, S = $[\sum(w(F_o^2 - F_c^2)^2)/(N_{diffrs} - N_{params})]^{½}$ for all data, $R(F) = \sum ||F_o| - |F_c|| / \sum |F_o|$ for observed data, $wR(F^2) = [\sum(w(F_o^2 - F_c^2)^2)/(\sum w(F_o^2)^2)]^{½}$ for all data.

3. IR and Raman spectra

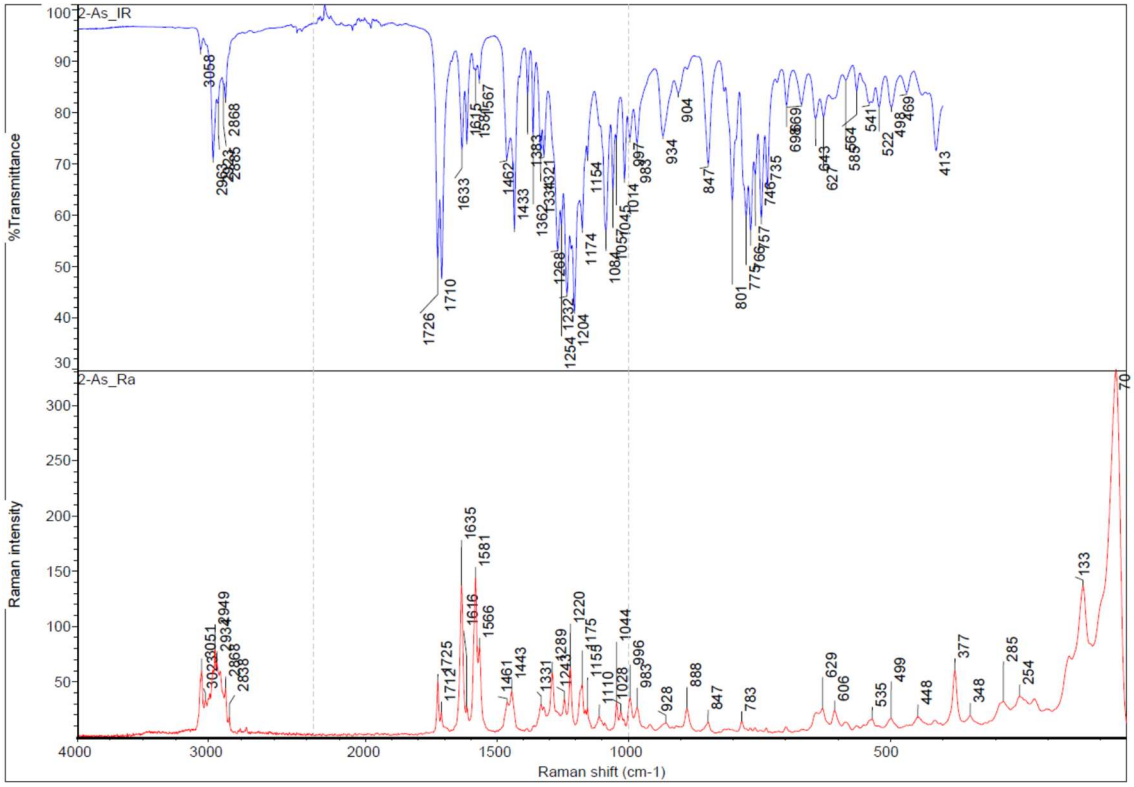


Figure S42: Infrared (top) and Raman (bottom) spectra of **2-As**.

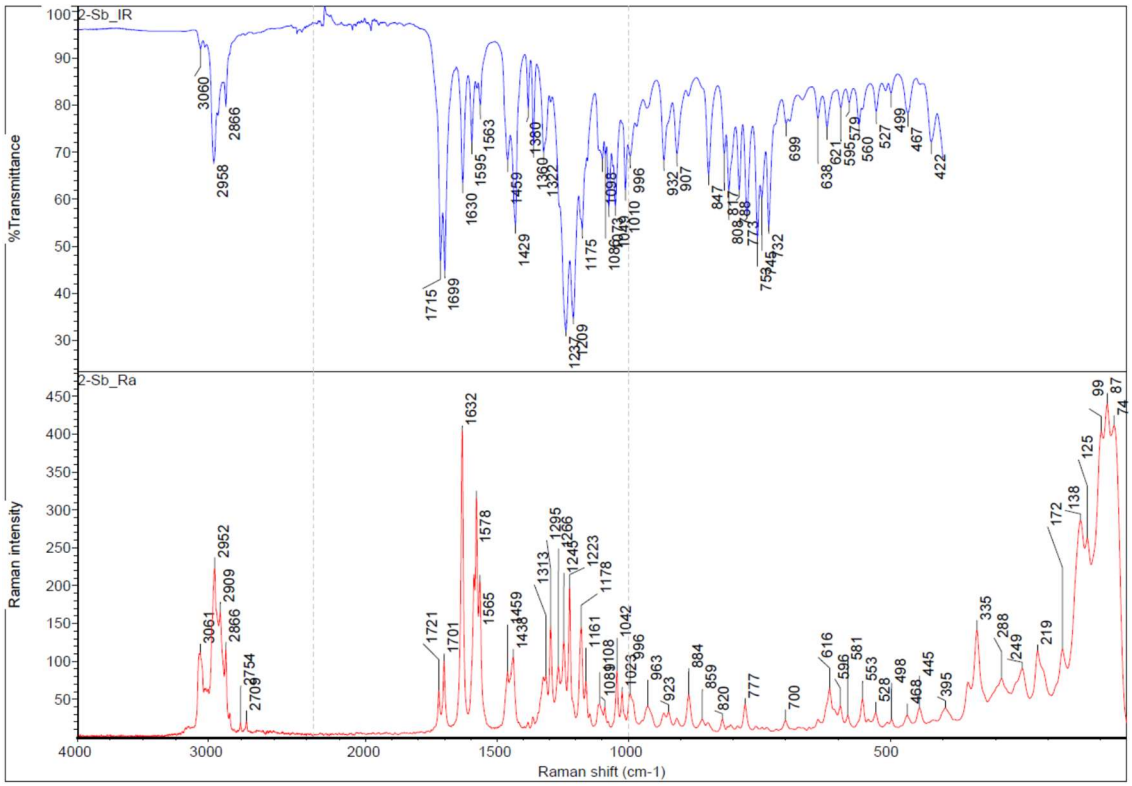


Figure S43: Infrared (top) and Raman (bottom) spectra of **2-Sb**.

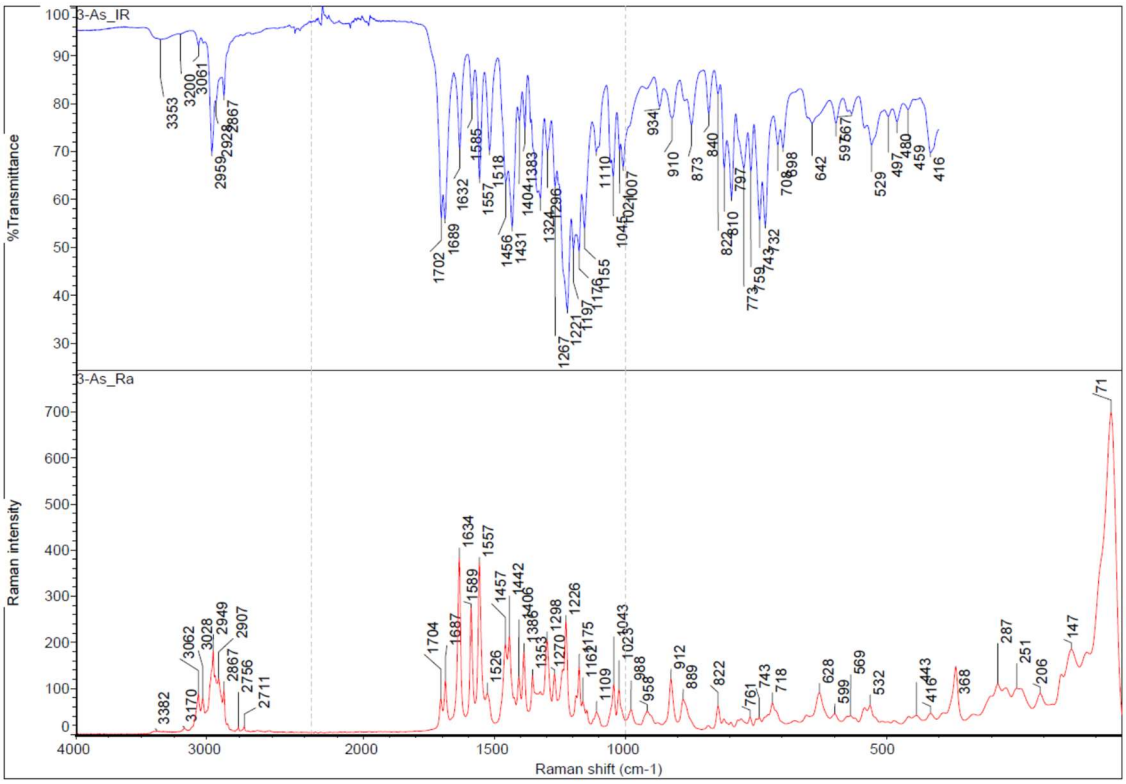


Figure S44: Infrared (top) and Raman (bottom) spectra of **3-As**.

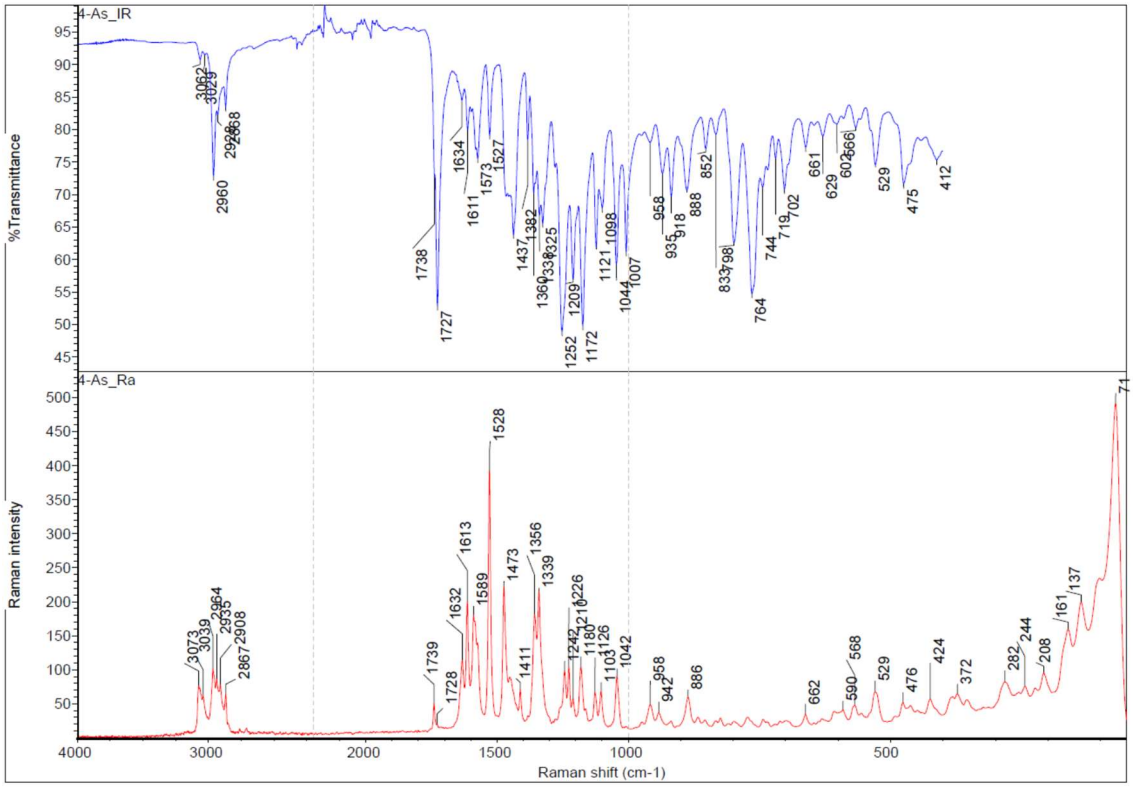


Figure S45: Infrared (top) and Raman (bottom) spectra of **4-As**.

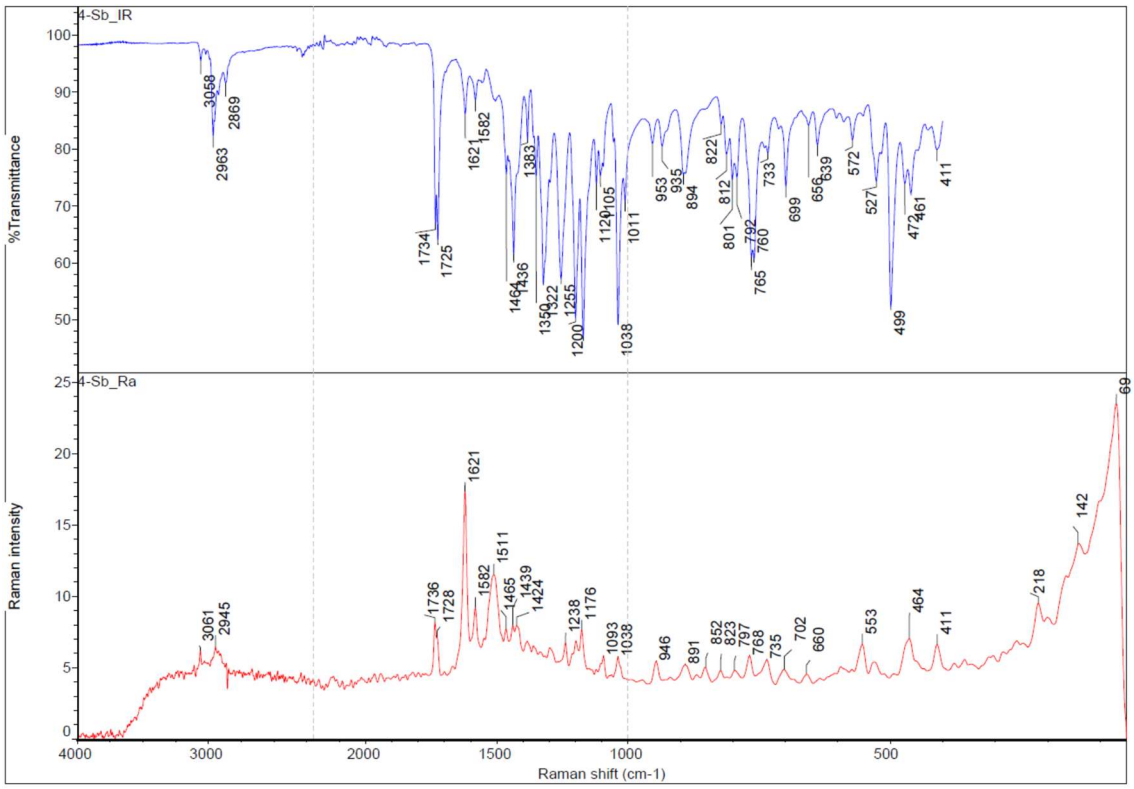


Figure S46: Infrared (top) and Raman (bottom) spectra of **4-Sb**.

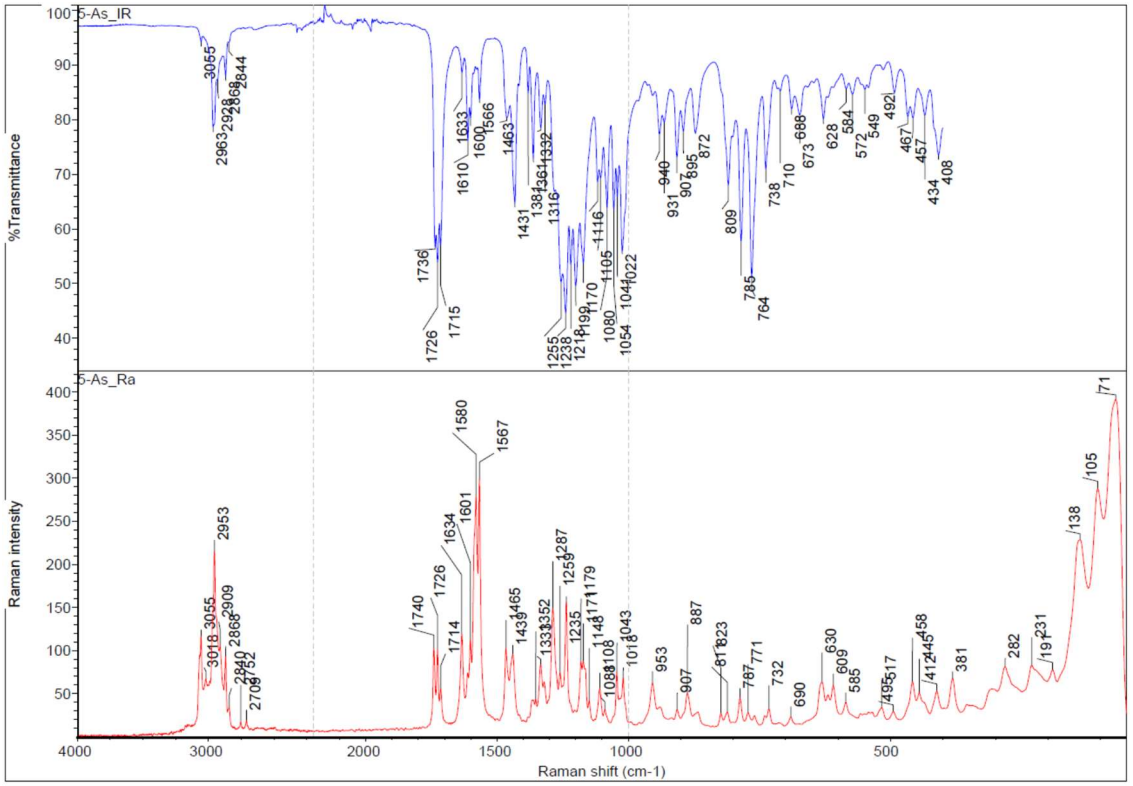


Figure S47: Infrared (top) and Raman (bottom) spectra of **5-As**.

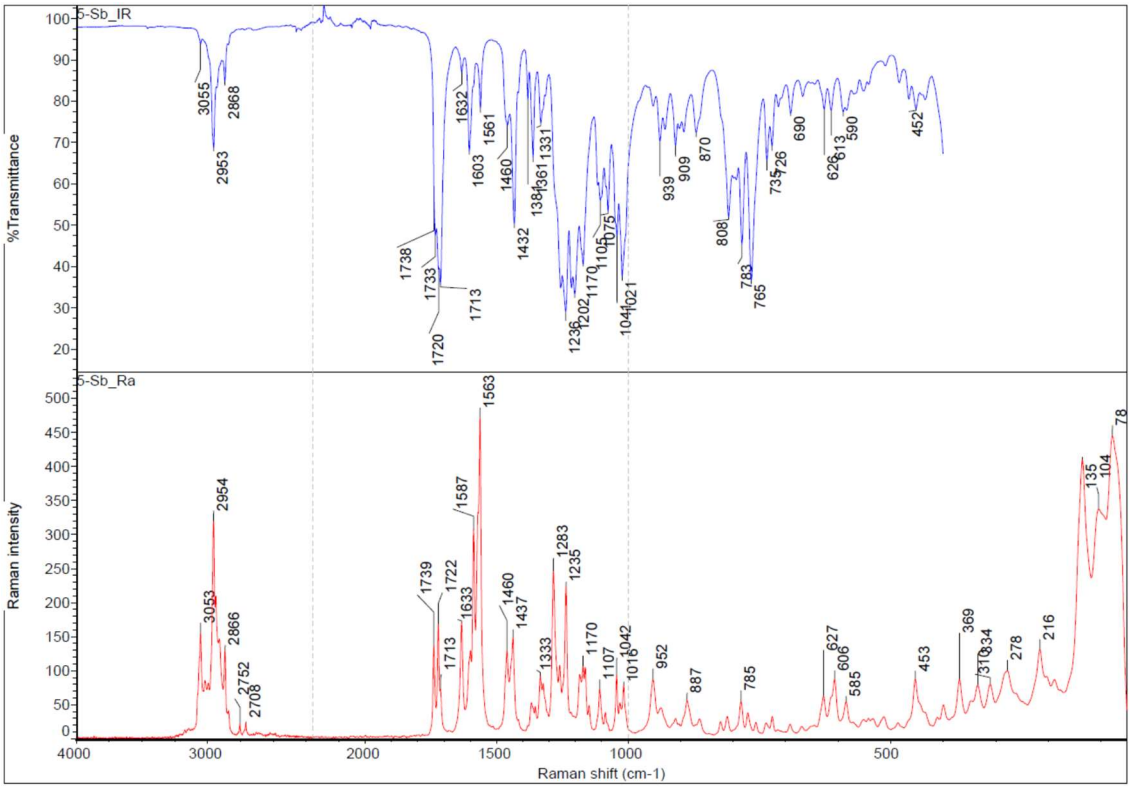


Figure S48: Infrared (top) and Raman (bottom) spectra of **5-Sb**.

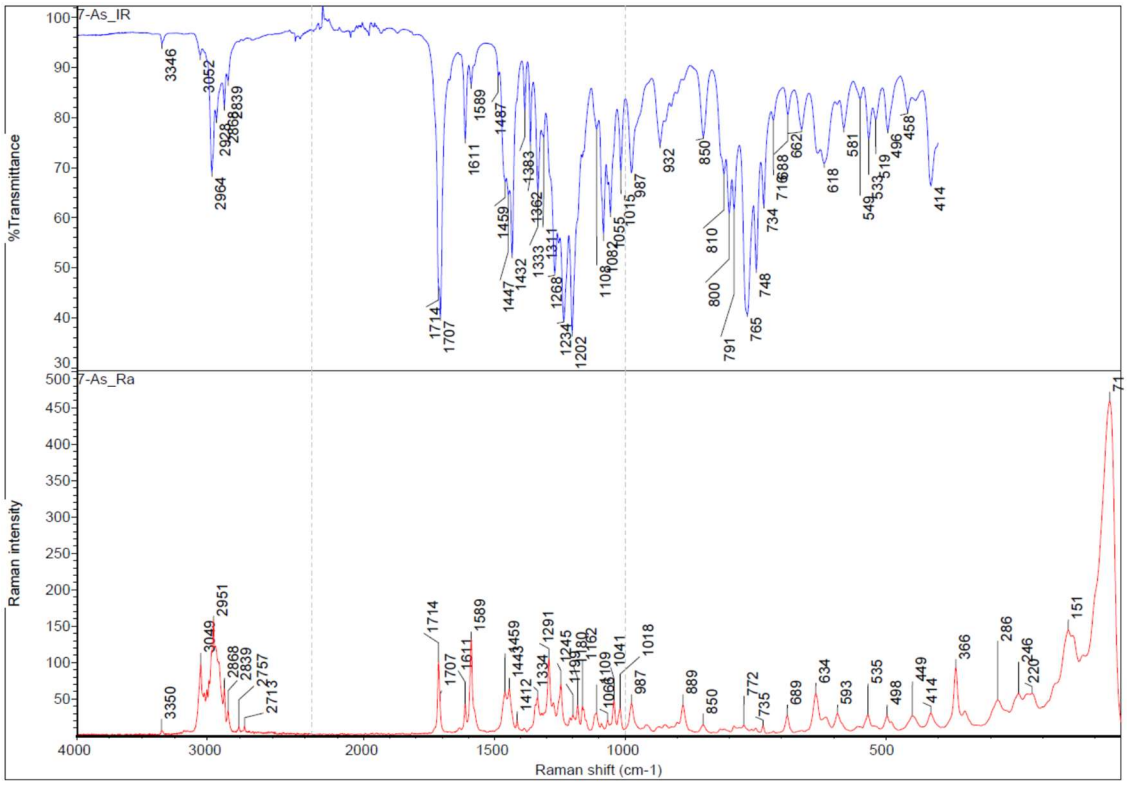


Figure S49: Infrared (top) and Raman (bottom) spectra of **7-As**.

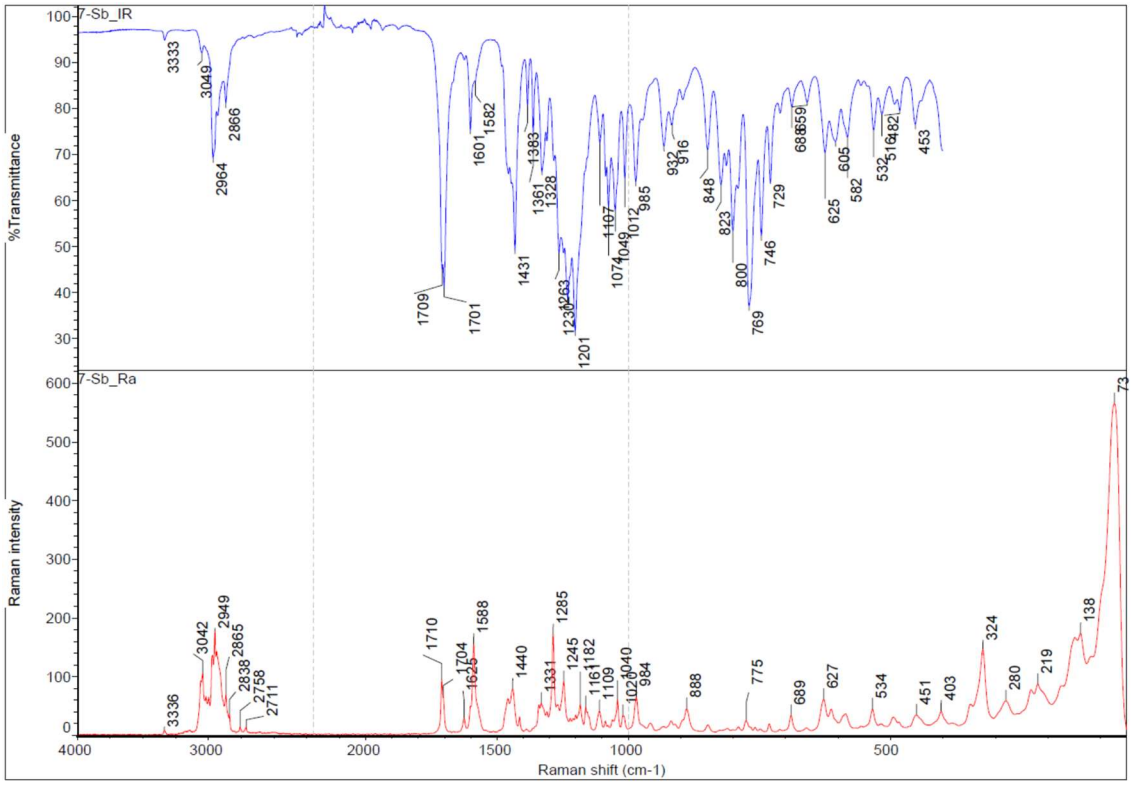


Figure S50: Infrared (top) and Raman (bottom) spectra of **7-Sb**.

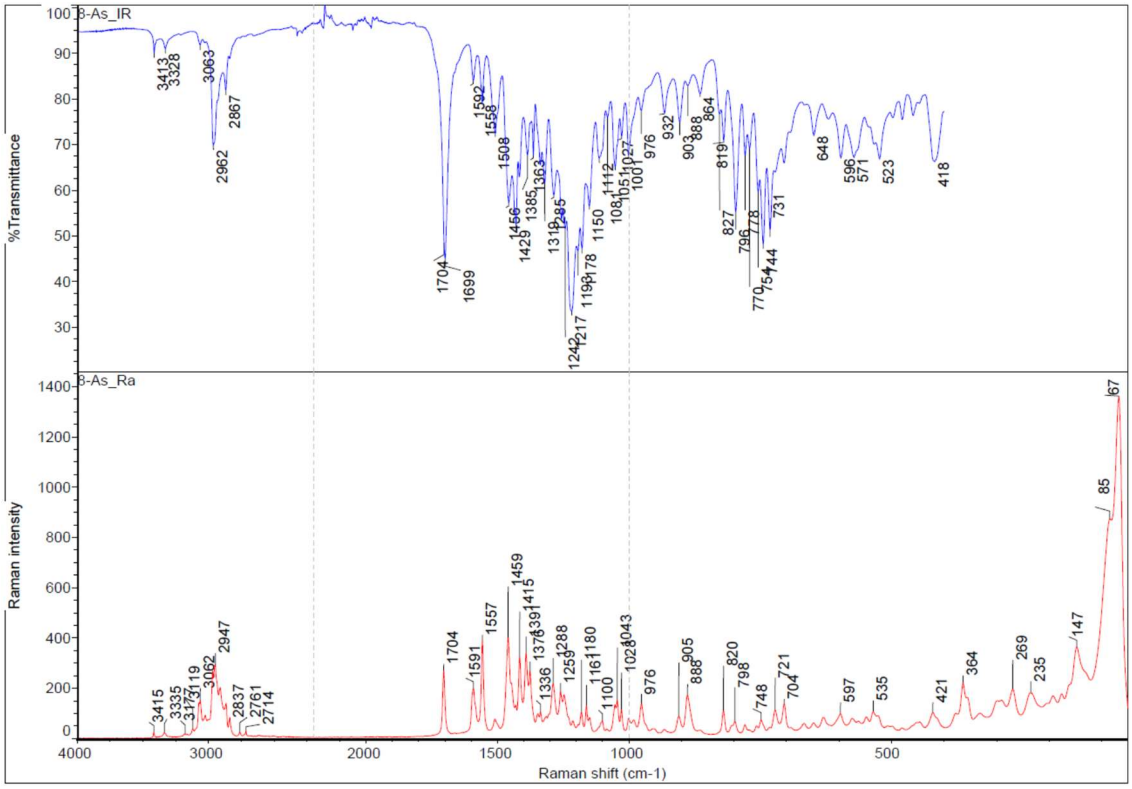


Figure S51: Infrared (top) and Raman (bottom) spectra of **8-As**.

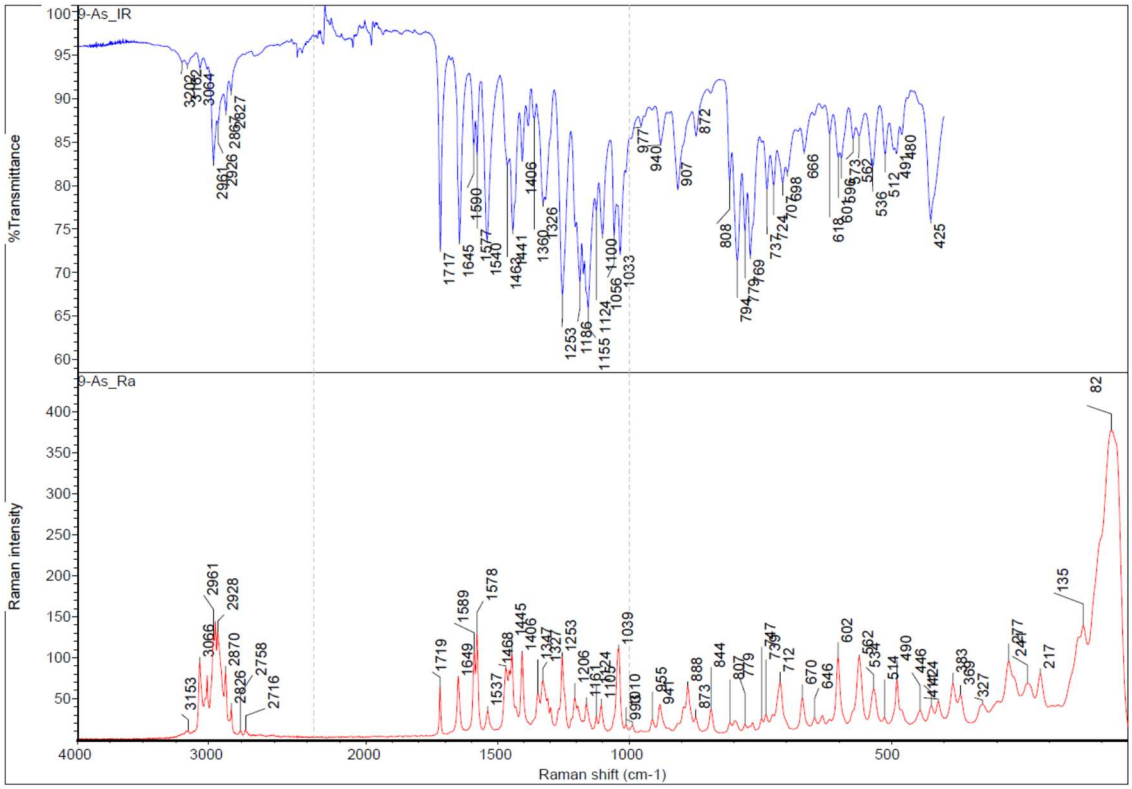


Figure S52 Infrared (top) and Raman (bottom) spectra of **9-As**.

4. Theoretical study

Table S2. Selected X-ray / DFT interatomic distances (Å) in the complexes studied.

Atoms	**2-As**	**2-Sb**	**7-Sb**
E(1)-C(1)	1.976(3) / 1.988	2.137(3) / 2.159	2.162(3) / 2.152
E(1)-N(1)	1.858(2) / 1.858	2.050(3) / 2.050	2.0447(19) / 2.035
E(1)-C(9)	2.013(3) / 2.022	2.203(3) / 2.211	2.196(3) / 2.210
E(1)-N(2)	3.015(2) / 3.006	2.907(3) / 2.982	3.123(2) / 3.221
C(8)-C(9)	1.333(4) / 1.327	1.331(4) / 1.329	1.332(3) / 1.328
C(7)-C(8)	1.553(4) / 1.538	1.556(5) / 1.541	1.545(3) / 1.549
C(2)-C(7)	1.528(4) / 1.534	1.539(5) / 1.536	1.524(4) / 1.531
Atoms	**4-Sb**	**5-As**	**5-Sb**
E(1)-C(1)	2.0438(19) / 2.058	1.963(6) / 1.982	2.136(4) / 2.151
E(1)-N(1)	2.3526(17) / 2.370	2.936(6) / 2.997	2.899(4) / 2.963
E(1)-N(2)	2.3370(17) / 2.333	1.874(6) / 1.861	2.057(4) / 2.052
C(8)-C(9)	1.330(3) / 1.332	1.335(11) / 1.330	1.333(8) / 1.330
C(7)-C(8)	1.493(3) / 1.489	1.514(9) / 1.503	1.508(6) / 1.500
N(1)-C(7)	1.313(3) / 1.297	- / -	- / -
N(2)-C(26)	1.297(3) / 1.290	- / -	- / -
E(1)-C(21)	- / -	2.015(7) / 2.027	2.211(6) / 2.209
C(21)-C(20)	- / -	1.334(9) / 1.328	1.357(6) / 1.329
C(22)-C(20)	- / -	1.542(10) / 1.541	1.547(7) / 1.543
Atoms	**8-As**	**9-As**	**10-Sb**
E(1)-C(1)	1.8971(17) / 1.907	1.921(2) / 1.930	- / 2.133
E(1)-C(9)	1.8300(18) / 1.830	2.046(2) / 2.046	- / -
E(1)-N(2)	- / -	1.849(2) / 1.856	- / 2.908
C(8)-C(9)	1.413(2) / 1.405	1.522(3) / 1.512	- / 1.329
C(7)-C(8)	1.404(2) / 1.396	1.395(3) / 1.391	- / -
C(2)-C(7)	1.451(2) / 1.450	1.493(4) / 1.488	- / -
C(1)-C(2)	1.419(2) / 1.415		- / -
C(1)-C(6)	- / -	1.394(3) / 1.381	- / -

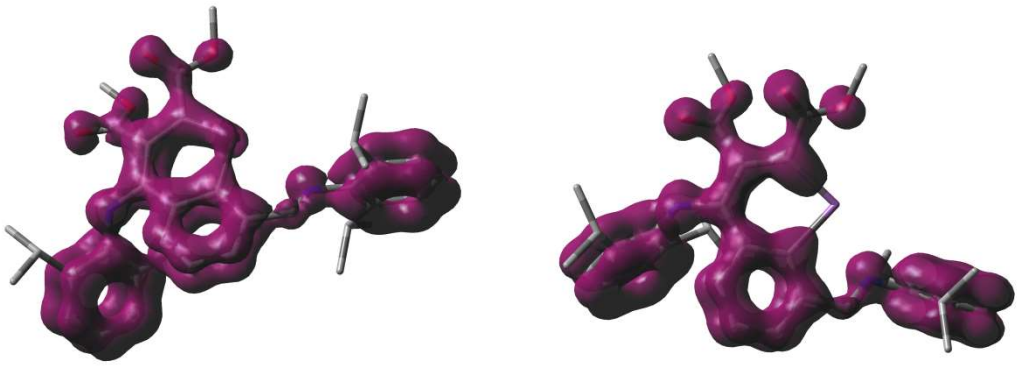
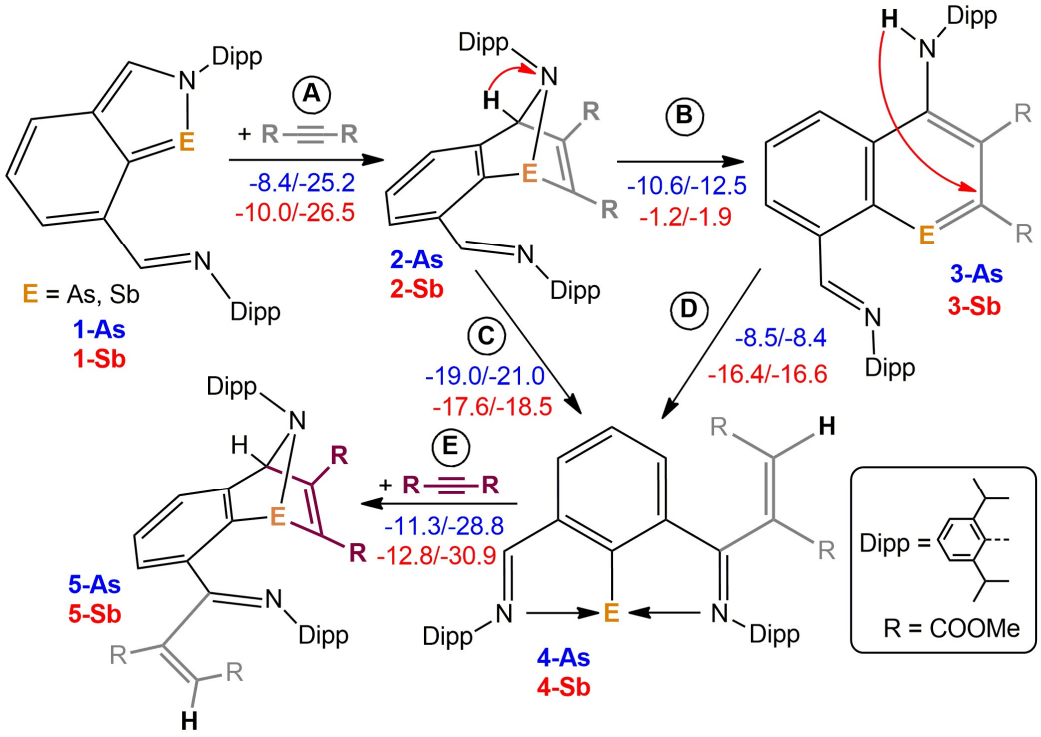
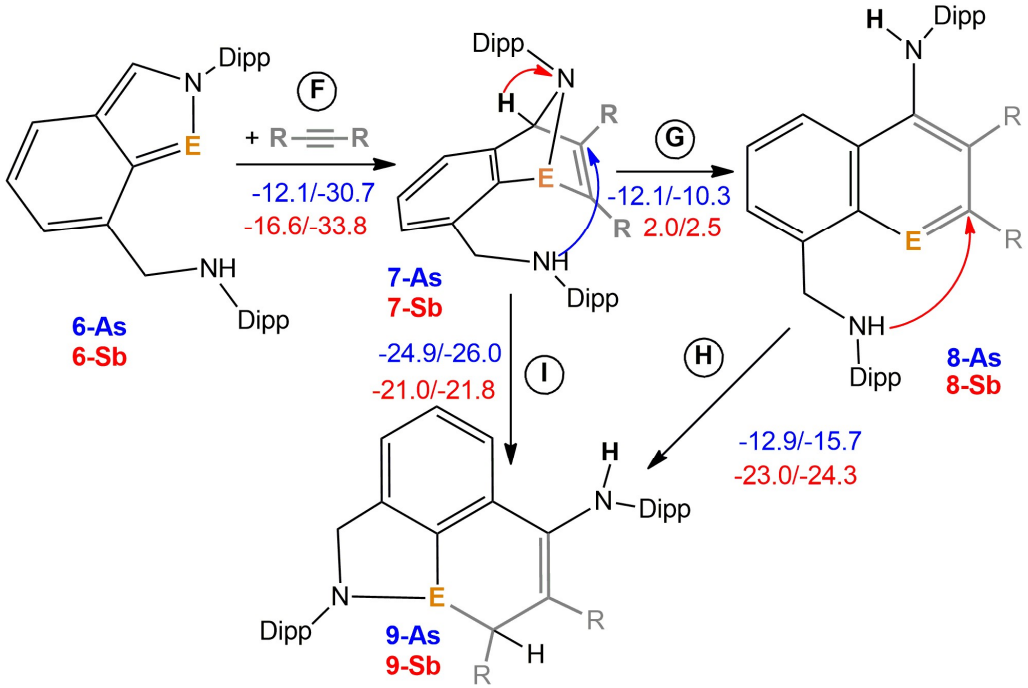


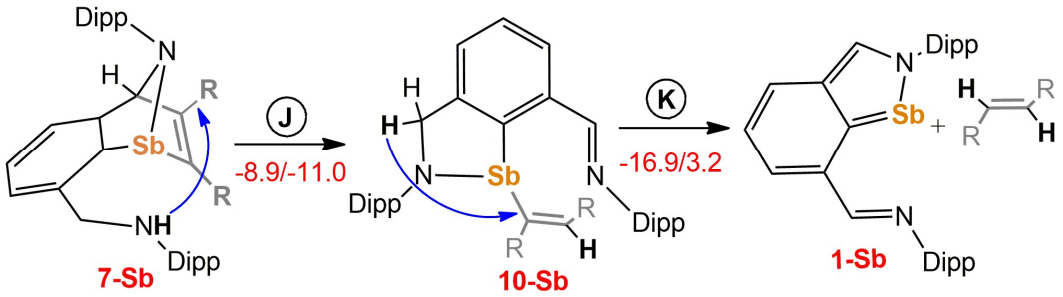
Figure S53. The $EDDB_H$ isosurfaces (isovalue 0.015 a.u.) of **3-As** (left) and **3-Sb** (right).



Scheme S1. Calculated $\Delta G^0/\Delta H^0$ values accompanying the reactions of **1-As** (blue) and **1-Sb** (red) with DMAD in C_6H_6 solution.



Scheme S2. Calculated $\Delta G^0/\Delta H^0$ values accompanying the reactions of **6-As** (blue) and **6-Sb** (red) with DMAD in C_6H_6 solution.



Scheme S2. Calculated $\Delta G^0/\Delta H^0$ values accompanying the reactions J and K in C_6H_6 solution.

Atomic coordinates (Å) in the optimized structures of the As and Sb complexes.

74
1-As

C	-1.258500	-1.024100	3.620200
H	-2.232900	-1.124300	4.085900
C	-1.181100	-0.634800	2.302400
C	-2.386600	-0.357500	1.530500
H	-3.354500	-0.480900	2.029200
N	-2.297200	0.016800	0.321500
C	0.084500	-0.499900	1.677100
C	-0.097200	-1.294500	4.374100
H	-0.189100	-1.598200	5.408000
C	1.138900	-1.173300	3.795200
H	2.037700	-1.380800	4.364500
C	1.246900	-0.776300	2.444600
C	2.440300	-0.610100	1.718000

H	3.439900	-0.764300	2.107800
N	2.264600	-0.234000	0.464700
C	3.371700	-0.008000	-0.413600
C	3.838100	-1.069300	-1.197900
C	3.929700	1.274200	-0.478600
C	4.896800	-0.816500	-2.065100
C	4.987200	1.475400	-1.360700
C	5.468200	0.442600	-2.148300
H	5.275500	-1.618000	-2.687700
H	5.437100	2.458400	-1.433800
H	6.289400	0.620000	-2.831000
C	-3.464300	0.258900	-0.438400
C	-3.773900	1.591000	-0.763100
C	-4.237500	-0.810000	-0.911800
C	-4.909200	1.836200	-1.523400
C	-5.367400	-0.512500	-1.671500
C	-5.710500	0.793900	-1.969400
H	-5.172400	2.854600	-1.778100
H	-5.985400	-1.322900	-2.039400
H	-6.593200	1.002900	-2.560200
C	3.416000	2.426700	0.361600
H	2.617000	2.054800	1.003900
C	2.819800	3.521700	-0.525200
H	2.011300	3.125000	-1.141000
H	2.419800	4.329700	0.089800
H	3.578300	3.944700	-1.187400
C	4.516200	2.989700	1.263200
H	4.934800	2.213600	1.905800
H	5.330800	3.414400	0.673400
H	4.114700	3.781700	1.897400
C	3.221200	-2.453000	-1.139100
H	2.463200	-2.457000	-0.354900
C	4.262800	-3.516600	-0.788400
H	3.783900	-4.491800	-0.688000
H	5.023200	-3.598600	-1.567400
H	4.765900	-3.282200	0.150900
C	2.521200	-2.786900	-2.458200
H	2.052200	-3.770500	-2.399200
H	1.749400	-2.050500	-2.686800
H	3.236000	-2.801300	-3.283900
C	-3.870300	-2.256600	-0.638000
H	-2.864100	-2.276700	-0.217700
C	-3.840500	-3.088500	-1.921400
H	-3.179100	-2.640900	-2.664000
H	-3.482900	-4.096600	-1.704800
H	-4.834800	-3.178700	-2.362200
C	-4.825800	-2.882200	0.380900
H	-4.820600	-2.332600	1.323500
H	-5.848800	-2.874700	-0.002400
H	-4.547200	-3.917800	0.584300

C	-2.900500	2.714400	-0.242700
H	-1.880400	2.324700	-0.186900
C	-2.887000	3.941900	-1.149100
H	-2.131100	4.647800	-0.801700
H	-2.657800	3.674400	-2.181400
H	-3.847100	4.461900	-1.135600
C	-3.327000	3.110400	1.174600
H	-4.353500	3.484900	1.166200
H	-3.281900	2.261700	1.858000
H	-2.678300	3.897300	1.564200
As	0.450600	0.005700	-0.086500

74

1-Sb

Sb	-0.000000	0.027500	-0.268600
C	-1.205700	-0.042600	3.900400
H	-2.144200	-0.053400	4.444000
C	-1.212200	-0.019300	2.507800
C	-2.405800	-0.013000	1.699700
H	-3.397500	-0.032800	2.153100
N	-2.258700	0.011200	0.420300
C	-0.000000	-0.005500	1.792600
C	-0.000000	-0.052800	4.595500
H	-0.000000	-0.070400	5.676500
C	1.205600	-0.042400	3.900400
H	2.144200	-0.053100	4.444000
C	1.212200	-0.019200	2.507800
C	2.405800	-0.012700	1.699700
H	3.397500	-0.032500	2.153100
N	2.258700	0.011500	0.420300
C	3.385300	0.005300	-0.449600
C	3.896300	-1.223200	-0.889600
C	3.911200	1.228500	-0.888300
C	4.982600	-1.202400	-1.759300
C	4.996100	1.196100	-1.758500
C	5.533100	-0.006400	-2.189100
H	5.403900	-2.138000	-2.105500
H	5.428100	2.126600	-2.104600
H	6.378900	-0.010900	-2.864600
C	-3.385300	0.005100	-0.449600
C	-3.911400	1.228300	-0.888000
C	-3.896000	-1.223400	-0.890100
C	-4.996300	1.196000	-1.758200
C	-4.982200	-1.202500	-1.759900
C	-5.533000	-0.006400	-2.189200
H	-5.428400	2.126600	-2.104000
H	-5.403400	-2.138000	-2.106500
H	-6.378800	-0.010900	-2.864800
C	3.354100	2.547800	-0.391300
H	2.343200	2.365000	-0.022400
C	3.256300	3.601900	-1.492500

H 2.704100 3.223000 -2.353300
H 2.738400 4.484400 -1.114200
H 4.242200 3.923200 -1.833200
C 4.196200 3.068100 0.777400
H 4.223600 2.349000 1.597800
H 5.224100 3.246900 0.452800
H 3.788800 4.006700 1.157700
C 3.321800 -2.540100 -0.405500
H 2.334100 -2.341800 0.014100
C 4.199100 -3.123600 0.705800
H 3.781000 -4.062500 1.073300
H 5.206000 -3.320800 0.330200
H 4.284600 -2.433300 1.546800
C 3.141800 -3.552000 -1.536300
H 2.623100 -4.436200 -1.162700
H 2.554800 -3.129200 -2.352500
H 4.101400 -3.881100 -1.939300
C -3.321400 -2.540200 -0.406200
H -2.333200 -2.342000 0.012500
C -3.142400 -3.552500 -1.537000
H -2.556300 -3.129800 -2.353900
H -2.623200 -4.436500 -1.163700
H -4.102400 -3.881900 -1.938900
C -4.197900 -3.123500 0.705800
H -4.282500 -2.433000 1.546800
H -5.205100 -3.320600 0.331100
H -3.779600 -4.062300 1.073200
C -3.354600 2.547600 -0.390500
H -2.343800 2.364700 -0.021200
C -3.256200 3.601700 -1.491700
H -2.738500 4.484300 -1.113000
H -2.703500 3.222900 -2.352200
H -4.241900 3.923000 -1.832900
C -4.197100 3.067800 0.777800
H -5.224900 3.246600 0.452700
H -4.224900 2.348600 1.598100
H -3.790000 4.006300 1.158400
90
2-As
As 0.156200 0.154600 -0.513600
O 3.724400 -2.392100 1.864000
N 1.893200 0.697800 -0.140200
C -0.070600 0.198900 1.460500
O 2.686700 -3.864800 0.530800
N -2.698300 -0.014900 0.412800
C 1.186800 0.101100 2.044500
C 1.331700 0.174700 3.416300
H 2.309100 0.086500 3.875300
O 0.830900 -3.273900 -1.981300
C 0.194000 0.369300 4.204200

H	0.293700	0.447100	5.279000
O	-0.535300	-3.542800	-0.224300
C	-1.060100	0.448100	3.623500
H	-1.939700	0.578800	4.243400
C	-1.207200	0.340600	2.234600
C	2.269100	-0.143400	0.985100
H	3.283000	0.033700	1.335500
C	0.942200	-1.692600	-0.272500
C	2.015000	-1.581200	0.500500
C	2.820700	-2.742400	0.943000
C	0.340600	-2.942700	-0.789900
C	4.544700	-3.454600	2.354000
H	3.926800	-4.219500	2.821600
H	5.213800	-3.003900	3.080000
H	5.108400	-3.900000	1.535700
C	0.297000	-4.473100	-2.548200
H	-0.781400	-4.383300	-2.672100
H	0.519000	-5.319200	-1.899700
H	0.785600	-4.588300	-3.510400
C	2.684900	1.765200	-0.620200
C	2.272900	3.101500	-0.450300
C	3.077500	4.117800	-0.957800
H	2.762400	5.148400	-0.849500
C	4.284200	3.839300	-1.576500
H	4.903900	4.645400	-1.948200
C	4.693200	2.524000	-1.717400
H	5.636600	2.308300	-2.205200
C	3.901200	1.472700	-1.268900
C	0.983600	3.464100	0.260900
H	0.657100	2.589100	0.822500
C	1.171800	4.591300	1.277700
H	0.252100	4.730000	1.848700
H	1.400700	5.540600	0.790600
H	1.978500	4.362900	1.975200
C	-0.114200	3.833800	-0.741100
H	-0.298600	3.030100	-1.456000
H	0.173900	4.722900	-1.307300
H	-1.050200	4.051100	-0.221300
C	4.359600	0.047100	-1.506000
H	3.538300	-0.614800	-1.235100
C	-2.541800	0.337300	1.617600
H	-3.388700	0.626400	2.251100
C	-3.981800	0.008400	-0.175300
C	-4.660800	1.214400	-0.396200
C	-5.920300	1.151200	-0.992100
H	-6.468000	2.070100	-1.165500
C	-6.477500	-0.055100	-1.373600
H	-7.458700	-0.079700	-1.830400
C	-5.765700	-1.233900	-1.190600
H	-6.195700	-2.172100	-1.517500

C	-4.509300	-1.223800	-0.603200
C	-4.060600	2.569700	-0.068600
H	-3.030800	2.419600	0.258500
C	-4.009500	3.466300	-1.308100
H	-5.012500	3.706400	-1.665400
H	-3.467600	2.979800	-2.120100
H	-3.507000	4.406600	-1.074000
C	-4.821800	3.261600	1.063600
H	-5.859700	3.441500	0.774600
H	-4.365700	4.225100	1.298900
H	-4.830300	2.653100	1.969100
C	-3.712100	-2.489000	-0.373300
H	-2.656400	-2.221700	-0.460800
C	-4.000500	-3.589400	-1.388800
H	-4.999300	-4.011300	-1.256200
H	-3.281400	-4.398800	-1.254200
H	-3.919000	-3.221000	-2.412900
C	-3.925600	-3.014600	1.049300
H	-4.966700	-3.317600	1.187200
H	-3.692300	-2.253400	1.794900
H	-3.283300	-3.877500	1.232300
C	5.572300	-0.305200	-0.640300
H	6.425500	0.325000	-0.902100
H	5.861600	-1.346600	-0.796200
H	5.366900	-0.164000	0.422100
C	4.669100	-0.207000	-2.983000
H	3.819100	0.058900	-3.612400
H	4.897600	-1.262200	-3.141900
H	5.532100	0.373800	-3.314300

90

2-Sb

Sb	-0.019400	0.163600	-0.697400
O	2.711700	-3.761200	0.886400
N	1.890300	0.745400	-0.229800
C	-0.176500	0.354600	1.447000
O	3.626100	-2.131700	2.119500
N	-2.773200	0.063200	0.442800
C	1.094500	0.284600	2.000300
C	1.266600	0.429800	3.367100
H	2.255000	0.365600	3.807300
O	-0.446000	-3.693400	-0.045300
C	0.149700	0.657900	4.173400
H	0.277700	0.790600	5.240000
O	1.052000	-3.551600	-1.706800
C	-1.122400	0.691900	3.624300
H	-1.988000	0.836500	4.260800
C	-1.292800	0.517200	2.247000
C	2.183300	-0.036800	0.964900
H	3.186100	0.148400	1.344600
C	1.957800	-1.515900	0.598200

C	0.930400	-1.771700	-0.204700
C	2.783300	-2.599500	1.192100
C	4.463900	-3.109400	2.737800
H	3.857300	-3.869900	3.226700
H	5.063400	-2.570000	3.464400
H	5.099800	-3.582400	1.990800
C	0.447400	-3.109600	-0.604300
C	0.650500	-4.851800	-2.141800
H	-0.411800	-4.859700	-2.382500
H	0.849400	-5.581800	-1.358500
H	1.244200	-5.065800	-3.024900
C	2.780300	1.750000	-0.666700
C	2.449000	3.114400	-0.537300
C	3.350100	4.072700	-0.992500
H	3.096500	5.122600	-0.910900
C	4.575200	3.711700	-1.527100
H	5.269400	4.472300	-1.861400
C	4.904800	2.370900	-1.632900
H	5.862500	2.088300	-2.054900
C	4.018900	1.377600	-1.229500
C	1.134700	3.561700	0.071700
H	0.726200	2.717500	0.627600
C	1.302800	4.705500	1.072700
H	1.614700	5.629400	0.582500
H	2.043600	4.457200	1.833800
H	0.352300	4.904400	1.570900
C	0.134100	3.957600	-1.018700
H	-0.011300	3.158200	-1.748100
H	0.496500	4.833400	-1.562400
H	-0.836200	4.205500	-0.582500
C	4.399700	-0.076900	-1.423700
H	3.525300	-0.681100	-1.186000
C	5.541200	-0.490900	-0.491200
H	5.767600	-1.552300	-0.614800
H	5.290800	-0.315600	0.556300
H	6.447300	0.075900	-0.718300
C	4.768600	-0.372600	-2.879300
H	3.966600	-0.073300	-3.555200
H	4.949200	-1.440800	-3.011800
H	5.675600	0.158100	-3.175000
C	-2.632700	0.431300	1.646700
H	-3.494200	0.659700	2.284300
C	-4.051700	-0.028100	-0.148500
C	-4.866800	1.099900	-0.316300
C	-6.106700	0.919700	-0.930200
H	-6.757700	1.775400	-1.065000
C	-6.517300	-0.322700	-1.375200
H	-7.486300	-0.438400	-1.843800
C	-5.676900	-1.419700	-1.235900
H	-5.996800	-2.385000	-1.605900

C -4.433500 -1.293700 -0.633800
C -4.443800 2.499800 0.090200
H -3.413300 2.462800 0.444100
C -4.470600 3.456200 -1.104900
H -3.840700 3.087700 -1.915500
H -4.107300 4.441200 -0.806600
H -5.483200 3.578300 -1.493000
C -5.315700 3.037200 1.227100
H -6.357700 3.112600 0.909000
H -4.982800 4.032100 1.527800
H -5.283200 2.383500 2.100200
C -3.509100 -2.477400 -0.438900
H -2.483300 -2.107500 -0.522900
C -3.691100 -3.578300 -1.478000
H -4.647400 -4.091500 -1.355900
H -2.901300 -4.320100 -1.352300
H -3.642500 -3.184900 -2.494900
C -3.658900 -3.057100 0.970800
H -4.664000 -3.465700 1.102200
H -3.498100 -2.296600 1.735600
H -2.929600 -3.853400 1.123500
90
3-As
As -1.061000 1.470000 -0.450200
H 4.092000 0.767900 -0.160900
N 3.394500 0.048700 -0.288400
O 4.007700 2.650100 0.396100
C -0.241000 -0.171700 -0.996300
O 2.371300 3.129700 1.834800
C 1.154800 -0.335200 -1.127500
C 1.650100 -1.395400 -1.925100
H 2.712800 -1.469200 -2.103200
O 1.238400 4.621000 -0.239500
C 0.810700 -2.308200 -2.505700
H 1.210100 -3.090700 -3.136400
O -0.790900 4.205900 0.601700
C -0.562000 -2.236400 -2.252500
H -1.229000 -2.995200 -2.645200
C 3.801800 -1.273200 0.036600
C 2.118000 0.526100 -0.462000
C 4.965700 -1.750200 -0.599800
C 5.404400 -3.034600 -0.311900
H 6.293400 -3.416700 -0.795500
C 4.706400 -3.845800 0.571000
H 5.050800 -4.851600 0.774600
C 3.575700 -3.357300 1.196300
H 3.044500 -3.985500 1.901300
C 3.108900 -2.063400 0.965600
C 5.724100 -0.855400 -1.560300
H 4.983300 -0.251000 -2.091800

C	6.648100	0.098300	-0.790900
H	7.415900	-0.475900	-0.267600
H	6.118700	0.694200	-0.045400
H	7.142400	0.787900	-1.477000
C	6.532100	-1.620600	-2.604700
H	7.381400	-2.137300	-2.153500
H	6.931300	-0.923100	-3.342000
H	5.920500	-2.358500	-3.126000
C	1.914500	-1.587800	1.775000
H	1.680900	-0.559700	1.508000
C	2.242600	-1.582800	3.271000
H	2.453400	-2.591000	3.632400
H	1.395000	-1.193100	3.837800
H	3.113100	-0.959800	3.480900
C	0.670400	-2.438500	1.500800
H	0.800000	-3.450400	1.891500
H	0.462100	-2.515000	0.432600
H	-0.203200	-1.999800	1.988200
C	1.793900	1.798100	-0.004200
C	0.502500	2.360200	-0.092800
C	2.846500	2.571800	0.723000
C	3.264800	4.011700	2.514700
H	2.726800	4.358800	3.391400
H	3.520300	4.846900	1.863200
H	4.171900	3.484200	2.804000
C	0.386200	3.834100	0.090400
C	-1.003500	5.613800	0.696400
H	-0.264800	6.060400	1.360500
H	-2.003500	5.735600	1.100700
H	-0.926100	6.075100	-0.287000
C	-2.516800	-1.282200	-1.185000
H	-3.111000	-1.956500	-1.814100
N	-3.029300	-0.675600	-0.202000
C	-4.405000	-0.822500	0.076700
C	-4.743300	-1.430900	1.299800
C	-5.385600	-0.323600	-0.791500
C	-6.086200	-1.580800	1.612100
C	-6.721700	-0.496700	-0.430100
C	-7.074900	-1.125400	0.749100
H	-6.370700	-2.054700	2.542500
H	-7.497600	-0.124200	-1.088500
H	-8.118900	-1.250800	1.006000
C	-5.053000	0.425300	-2.068500
H	-3.972700	0.565400	-2.116100
C	-5.684700	1.819500	-2.074900
H	-5.386500	2.388000	-1.193400
H	-5.370900	2.370700	-2.963000
H	-6.774600	1.759800	-2.088100
C	-5.485700	-0.364800	-3.305300
H	-5.008200	-1.345300	-3.339900

H -6.566400 -0.522100 -3.302400
H -5.226100 0.177700 -4.216000
C -3.642900 -1.944700 2.205900
H -2.806700 -1.245800 2.110100
C -3.156700 -3.320200 1.735400
H -2.348500 -3.680100 2.375200
H -3.975500 -4.042300 1.779400
H -2.786700 -3.286600 0.709800
C -4.045500 -2.008300 3.676100
H -3.173100 -2.245100 4.286800
H -4.458500 -1.059400 4.021000
H -4.787600 -2.789300 3.854300
C -1.081600 -1.205700 -1.499200
90
3-Sb
H 4.153300 0.662100 -0.339800
N 3.435500 -0.046300 -0.374800
O 4.119600 2.583900 0.148800
C -0.216900 -0.355500 -0.973200
O 2.588900 3.033000 1.708300
C 1.181400 -0.458000 -1.140700
C 1.698200 -1.535100 -1.905700
H 2.757500 -1.567200 -2.114700
O 1.464800 4.589400 -0.320300
C 0.890300 -2.519500 -2.411300
H 1.312300 -3.314200 -3.011600
O -0.606400 4.277000 0.462300
C -0.475300 -2.499800 -2.120500
H -1.117800 -3.308000 -2.450800
C 3.824200 -1.336600 0.068600
C 2.154200 0.445800 -0.535400
C 4.970500 -1.893000 -0.535900
C 5.400900 -3.147200 -0.126800
H 6.277800 -3.587700 -0.582300
C 4.711400 -3.857400 0.845000
H 5.050400 -4.840200 1.145900
C 3.594100 -3.296000 1.431800
H 3.068800 -3.843700 2.205100
C 3.135600 -2.027100 1.078400
C 5.724600 -1.113300 -1.595500
H 4.986900 -0.538400 -2.163000
C 6.695600 -0.119400 -0.944400
H 7.447800 -0.663300 -0.368800
H 6.197900 0.574200 -0.264200
H 7.206800 0.470500 -1.707000
C 6.477900 -1.999200 -2.584100
H 7.327400 -2.495600 -2.111500
H 6.869900 -1.389400 -3.398800
H 5.828500 -2.765600 -3.009900
C 1.954500 -1.468100 1.853700

H	1.705200	-0.478200	1.479900
C	2.311000	-1.294400	3.333000
H	2.544100	-2.254200	3.797600
H	1.470000	-0.853400	3.871400
H	3.176500	-0.641200	3.453000
C	0.713300	-2.351700	1.697100
H	0.845500	-3.303900	2.216100
H	0.506400	-2.568000	0.648000
H	-0.162500	-1.855800	2.122700
C	1.874800	1.741100	-0.114100
C	0.611200	2.365800	-0.171700
C	2.985200	2.497700	0.554700
C	3.529600	3.902400	2.337900
H	3.047500	4.253600	3.245000
H	3.756300	4.736000	1.673900
H	4.446200	3.364700	2.574000
C	0.573200	3.836300	-0.009500
C	-0.752100	5.693400	0.532200
H	-0.005400	6.115600	1.203200
H	-1.752200	5.870000	0.916400
H	-0.635800	6.137200	-0.455600
C	-2.438200	-1.544700	-1.063100
H	-3.010000	-2.339300	-1.556900
N	-2.968500	-0.788000	-0.198700
C	-4.338000	-0.915200	0.123100
C	-4.649300	-1.331200	1.430000
C	-5.336700	-0.572500	-0.797800
C	-5.985600	-1.451400	1.781900
C	-6.664900	-0.705300	-0.393600
C	-6.992200	-1.148300	0.874100
H	-6.250500	-1.779600	2.778600
H	-7.455900	-0.450000	-1.088900
H	-8.030500	-1.246300	1.163600
C	-5.033700	-0.026500	-2.180900
H	-3.954100	0.090200	-2.279900
C	-5.653400	1.359500	-2.374400
H	-5.314400	2.049600	-1.600900
H	-5.370300	1.765600	-3.347000
H	-6.743200	1.313800	-2.335200
C	-5.504200	-0.986400	-3.275500
H	-5.039100	-1.968000	-3.171100
H	-6.586500	-1.124500	-3.229700
H	-5.257300	-0.590300	-4.262000
C	-3.529200	-1.682100	2.388000
H	-2.695700	-1.011400	2.157500
C	-3.050200	-3.118300	2.149300
H	-2.232500	-3.368000	2.828300
H	-3.868700	-3.819700	2.326600
H	-2.696000	-3.259700	1.127100
C	-3.900700	-1.489700	3.855100

H -3.012900 -1.607500 4.478100
H -4.318200 -0.498400 4.036100
H -4.629200 -2.233300 4.185100
C -1.015200 -1.447100 -1.411000
Sb -1.186300 1.435700 -0.407400
90
4-As
O -5.067600 -0.968600 -0.897800
N -1.250200 -0.500000 0.083400
C 0.577900 0.791300 -1.056200
O -3.364000 -1.666300 -2.174700
N 3.216000 0.413700 -0.213300
C -0.730600 1.053700 -1.532300
O -4.414200 3.794500 -0.852600
C -0.931100 1.944800 -2.609000
H -1.934500 2.124100 -2.976900
C 0.140300 2.567800 -3.190300
H -0.008400 3.248600 -4.017200
O -2.390700 3.170400 -0.131400
C 1.445900 2.320200 -2.716700
H 2.288500 2.817500 -3.184200
C 1.670200 1.452600 -1.673900
C -1.729000 0.333400 -0.843500
C -2.848400 -0.621100 1.925000
C -2.130100 -1.276100 0.913300
C -3.729900 -1.376300 2.692100
H -4.293100 -0.893100 3.480700
C -3.887300 -2.733500 2.471200
H -4.578700 -3.305400 3.077100
C -3.147300 -3.364100 1.484900
H -3.264400 -4.429600 1.332900
C -2.251600 -2.657000 0.686300
C -2.636200 0.843500 2.252000
H -2.102500 1.318600 1.430700
C -3.950900 1.600100 2.447200
H -3.752100 2.671800 2.505100
H -4.449200 1.306600 3.373200
H -4.644500 1.419600 1.623300
C -1.756700 0.967800 3.500700
H -0.795200 0.474100 3.351200
H -2.248100 0.509700 4.362400
H -1.571000 2.018800 3.728600
C -1.416400 -3.393700 -0.343200
H -1.032700 -2.660600 -1.054200
C -2.210900 -4.434900 -1.132300
H -3.095900 -3.997000 -1.590400
H -2.512500 -5.273100 -0.501300
H -1.583300 -4.840000 -1.927600
C -0.228300 -4.074100 0.347500
H 0.406600 -4.565100 -0.392400

H	-0.586300	-4.832400	1.048200
H	0.381500	-3.361300	0.901800
C	-3.179900	0.435600	-1.073200
C	-3.920400	1.546000	-1.035600
H	-4.975800	1.482300	-1.266500
C	-3.449900	2.894000	-0.626700
C	-4.104900	5.132500	-0.460000
H	-3.224300	5.486600	-0.993800
H	-3.913500	5.173600	0.611400
H	-4.976000	5.726300	-0.717500
C	-3.862700	-0.852300	-1.445700
C	-5.754300	-2.191700	-1.178900
H	-5.878700	-2.318100	-2.253100
H	-6.717000	-2.109500	-0.684700
H	-5.186100	-3.028700	-0.773400
C	3.022600	1.191100	-1.197400
H	3.851800	1.683300	-1.717400
C	4.531100	0.114400	0.207600
C	5.367200	-0.686800	-0.582900
C	6.645600	-0.968400	-0.103700
H	7.310300	-1.579300	-0.703200
C	7.076600	-0.492900	1.120900
H	8.073500	-0.724200	1.473700
C	6.219900	0.268500	1.905300
H	6.558100	0.621400	2.871000
C	4.938600	0.577900	1.471500
C	4.921900	-1.276800	-1.908300
H	3.855400	-1.085700	-2.028500
C	5.657800	-0.621900	-3.079500
H	5.496400	0.457000	-3.099000
H	5.315700	-1.038500	-4.028700
H	6.733500	-0.795200	-3.000900
C	5.110700	-2.795000	-1.939800
H	6.166800	-3.067200	-1.893200
H	4.704200	-3.203400	-2.866700
H	4.600800	-3.270900	-1.101400
C	3.996400	1.434500	2.292100
H	2.983800	1.072200	2.093500
C	4.065900	2.894500	1.831300
H	3.361900	3.508300	2.396400
H	3.827400	2.991400	0.771800
H	5.071700	3.290200	1.991100
C	4.245100	1.347200	3.794700
H	5.183800	1.830300	4.074000
H	4.278100	0.311800	4.136600
H	3.444700	1.859700	4.330100
As	0.633400	-0.437300	0.347900

90
4-Sb

Sb	1.039500	-0.443100	0.326500

O	-5.168500	-0.815900	-0.872900
N	-1.319700	-0.475200	0.104900
C	0.567600	0.755700	-1.278000
O	-3.495300	-1.556000	-2.168100
N	3.062000	0.368400	-0.507400
C	-0.769800	0.974500	-1.651900
O	-4.259200	3.914100	-0.647600
C	-1.060500	1.769100	-2.758100
H	-2.090600	1.927100	-3.056300
C	-0.036400	2.362200	-3.489200
H	-0.274600	2.974700	-4.348000
O	-2.220100	3.162200	-0.114600
C	1.289500	2.171900	-3.115900
H	2.087200	2.643400	-3.679700
C	1.595400	1.373800	-2.017000
C	-1.759000	0.317800	-0.823400
C	-2.903000	-0.490300	1.974700
C	-2.230600	-1.178200	0.951600
C	-3.808200	-1.199600	2.758100
H	-4.336000	-0.685700	3.552100
C	-4.038600	-2.547700	2.545900
H	-4.752200	-3.081200	3.160800
C	-3.335900	-3.217700	1.557400
H	-3.500800	-4.278400	1.414600
C	-2.414700	-2.558200	0.749100
C	-2.606800	0.960300	2.296500
H	-2.074000	1.406400	1.459600
C	-3.871200	1.786500	2.535600
H	-3.615000	2.847000	2.579200
H	-4.349000	1.525500	3.481900
H	-4.606500	1.639500	1.741300
C	-1.677700	1.037200	3.512400
H	-0.742700	0.508400	3.319500
H	-2.153600	0.589200	4.387900
H	-1.441000	2.077700	3.742800
C	-1.602800	-3.341700	-0.264800
H	-1.175200	-2.634500	-0.977200
C	-2.430800	-4.355500	-1.054700
H	-3.278000	-3.880100	-1.546000
H	-2.796100	-5.160900	-0.414500
H	-1.806400	-4.812700	-1.824000
C	-0.455000	-4.064200	0.450600
H	0.182600	-4.573300	-0.274900
H	-0.854400	-4.811100	1.141500
H	0.165100	-3.372900	1.020900
C	-3.222500	0.507300	-1.024300
C	-3.905100	1.646200	-0.917800
H	-4.972900	1.641100	-1.094100
C	-3.332900	2.958900	-0.519200
C	-3.843000	5.224700	-0.259400

H	-2.980000	5.534000	-0.846600
H	-3.578600	5.234700	0.797300
H	-4.691500	5.874000	-0.449300
C	-3.961200	-0.738900	-1.420600
C	-5.901100	-2.009000	-1.167400
H	-6.025000	-2.121900	-2.243100
H	-6.862100	-1.893300	-0.676800
H	-5.367200	-2.869800	-0.765300
C	2.931300	1.125200	-1.543200
H	3.800100	1.562100	-2.035800
C	4.341100	0.104000	0.056900
C	5.001200	-1.087400	-0.270400
C	6.229700	-1.339500	0.333900
H	6.759000	-2.254600	0.096100
C	6.784200	-0.443800	1.232900
H	7.741900	-0.656100	1.690700
C	6.106700	0.722400	1.550500
H	6.543000	1.416700	2.258200
C	4.872700	1.016500	0.980300
C	4.412900	-2.094400	-1.239500
H	3.488400	-1.679900	-1.643000
C	5.357800	-2.362500	-2.412000
H	5.609000	-1.438900	-2.935600
H	4.891700	-3.045900	-3.123800
H	6.288800	-2.820300	-2.071500
C	4.055800	-3.396100	-0.518700
H	4.946500	-3.860200	-0.089100
H	3.607200	-4.104900	-1.217300
H	3.343300	-3.213100	0.287400
C	4.151500	2.300300	1.343500
H	3.125900	2.228800	0.978700
C	4.815700	3.498600	0.660200
H	4.281200	4.419800	0.897900
H	4.829200	3.378800	-0.424400
H	5.849100	3.605800	0.998500
C	4.078800	2.512800	2.855600
H	5.068000	2.673400	3.288000
H	3.625400	1.652900	3.350200
H	3.474800	3.393700	3.078800

106

5-As

As	0.986000	-0.130900	-0.624600
O	1.628600	-3.219700	-1.783600
N	2.523400	0.731200	-0.028500
C	0.368200	0.127300	1.240900
N	-1.926700	-0.673300	-0.174500
O	1.568600	-4.141900	0.257900
C	1.488100	0.265500	2.050900
O	4.335400	-3.224900	0.960100
C	1.355800	0.492000	3.406900

H	2.229000	0.575000	4.042300
O	4.073600	-2.035400	2.842000
C	0.071800	0.607200	3.942400
H	-0.052200	0.792400	5.001400
O	-3.416000	4.121500	1.510400
C	-1.046800	0.477400	3.136200
H	-2.036400	0.556700	3.569600
C	-0.905600	0.219100	1.768800
O	-1.678300	2.887700	0.823400
C	2.778300	0.087300	1.247200
H	3.666100	0.459700	1.753500
O	-5.654300	-0.150500	1.026700
C	3.330900	1.757800	-0.565500
O	-4.234300	-1.521100	2.089600
C	2.816400	3.064100	-0.685000
C	3.644700	4.063800	-1.186000
H	3.259000	5.070200	-1.291000
C	4.959700	3.801400	-1.533200
H	5.594400	4.597500	-1.901300
C	4.652900	1.473200	-0.959900
C	5.455600	2.514100	-1.415900
H	6.480600	2.309100	-1.701900
C	1.383500	3.390800	-0.316400
H	1.016100	2.609600	0.350200
C	1.243900	4.713800	0.434900
H	1.454500	5.570900	-0.207800
H	1.916500	4.757100	1.292800
H	0.218500	4.808000	0.793600
C	0.501900	3.401900	-1.569000
H	0.827900	4.190800	-2.252600
H	-0.540300	3.580600	-1.294600
H	0.556500	2.453300	-2.106600
C	5.211300	0.064200	-0.924400
H	4.376800	-0.616100	-0.764200
C	2.834300	-1.420000	0.930200
C	1.942900	-1.797300	0.021300
C	1.701600	-3.178900	-0.448500
C	1.423400	-4.515400	-2.349100
H	1.373700	-4.364800	-3.422900
H	0.494700	-4.944400	-1.977200
H	2.253200	-5.171600	-2.090200
C	3.793400	-2.255500	1.691200
C	5.238300	-4.087000	1.655300
H	5.594100	-4.799100	0.917800
H	4.717900	-4.598300	2.463400
H	6.066300	-3.510500	2.065900
C	-2.073000	0.010900	0.885700
C	-3.031900	-0.901900	-1.033500
C	-3.505500	0.104300	-1.883800
C	-4.604500	-0.188400	-2.691000

H -4.986900 0.574800 -3.358400
C -5.212200 -1.429300 -2.655100
H -6.073000 -1.632100 -3.279600
C -4.702900 -2.424800 -1.830200
H -5.173000 -3.399500 -1.820900
C -3.598900 -2.190500 -1.022400
C -2.816500 1.449200 -2.009900
H -2.095700 1.555800 -1.198800
C -2.032900 1.506200 -3.325300
H -1.258500 0.737100 -3.351200
H -1.555200 2.480600 -3.442800
H -2.700700 1.347700 -4.175100
C -3.793100 2.623200 -1.922500
H -4.416400 2.688100 -2.816700
H -3.239200 3.561600 -1.838700
H -4.457700 2.533800 -1.060900
C -2.965600 -3.279900 -0.180900
H -2.645200 -2.829500 0.759400
C -1.719100 -3.809200 -0.898300
H -2.004000 -4.304000 -1.830600
H -1.189200 -4.526900 -0.269000
H -1.033900 -2.994000 -1.141100
C -3.913200 -4.423300 0.160800
H -4.189300 -4.998600 -0.725500
H -4.824500 -4.053900 0.634500
H -3.425400 -5.107900 0.855600
C -3.419200 0.555300 1.272100
C -3.747700 1.835000 1.422500
H -4.765400 2.101900 1.677300
C -2.812600 2.968700 1.217400
C -2.626100 5.296500 1.322700
H -1.776500 5.287900 2.004100
H -3.281500 6.133600 1.539600
H -2.263700 5.344800 0.296100
C -4.466700 -0.495000 1.508600
C -6.681000 -1.137000 1.170600
H -7.569600 -0.704500 0.722600
H -6.845200 -1.360600 2.223200
H -6.387200 -2.044000 0.642600
C 6.216700 -0.123900 0.215100
H 6.586800 -1.151400 0.230300
H 5.778700 0.093400 1.190800
H 7.072200 0.542600 0.081200
C 5.848000 -0.329900 -2.259200
H 6.750300 0.249600 -2.462700
H 5.152500 -0.176200 -3.085100
H 6.129900 -1.384100 -2.238900
106
5-Sb
Sb -0.837100 -0.191500 -0.831800

O	3.473600	4.155800	1.576000
N	2.012100	-0.620900	-0.141400
C	-0.276300	0.177400	1.211900
O	1.787900	2.920900	0.772000
N	-2.527700	0.735600	-0.128800
C	0.976200	0.291300	1.782700
O	5.734900	-0.130100	1.108700
C	1.079300	0.576600	3.146200
H	2.053100	0.673100	3.611400
O	4.286800	-1.491900	2.144800
C	-0.070800	0.708600	3.909700
H	0.012900	0.915000	4.968900
O	-1.677400	-3.496900	-1.640100
C	-1.333600	0.565700	3.333600
H	-2.227300	0.646600	3.940900
C	-1.426300	0.313100	1.975200
O	-1.629900	-4.230600	0.476200
C	2.156600	0.063200	0.921100
O	-4.365900	-3.158000	1.064300
C	3.114800	-0.891400	-0.991700
O	-4.011700	-1.901600	2.885900
C	3.638200	-2.198200	-0.962800
C	4.732200	-2.479400	-1.769400
H	5.170900	-3.468400	-1.748600
C	5.271300	-1.512400	-2.609500
H	6.123600	-1.752100	-3.232600
C	4.705700	-0.252300	-2.661600
H	5.112100	0.488600	-3.340000
C	3.618900	0.087500	-1.856200
C	2.972600	-3.254000	-0.102400
H	2.666300	-2.777000	0.829200
C	1.710200	-3.766700	-0.805500
H	1.048000	-2.941400	-1.076600
H	1.159200	-4.446900	-0.152900
H	1.977100	-4.299200	-1.722000
C	3.889000	-4.415200	0.263500
H	3.381100	-5.073400	0.969200
H	4.807600	-4.059700	0.733800
H	4.153400	-5.014100	-0.610600
C	2.976700	1.453900	-1.993700
H	2.251100	1.584600	-1.190500
C	2.210700	1.541900	-3.317600
H	2.889000	1.405000	-4.162800
H	1.732700	2.518600	-3.416300
H	1.437500	0.773700	-3.375400
C	3.991700	2.593600	-1.892500
H	4.637000	2.627800	-2.772500
H	4.632700	2.486300	-1.015300
H	3.470800	3.551900	-1.828300
C	3.502700	0.592600	1.319000

C	3.832100	1.873100	1.460700
H	4.845400	2.142000	1.730200
C	2.898300	3.004400	1.228800
C	2.678800	5.326400	1.377500
H	2.354900	5.388200	0.338900
H	3.316300	6.166200	1.633600
H	1.804200	5.297100	2.025700
C	4.537500	-0.465500	1.572200
C	6.749400	-1.128200	1.262200
H	6.895300	-1.359400	2.315900
H	7.649100	-0.702400	0.830200
H	6.453600	-2.029000	0.724800
C	-2.715500	0.103300	1.168400
H	-3.591900	0.476700	1.695400
C	-3.360000	1.791600	-0.551600
C	-2.852600	3.104800	-0.641500
C	-3.704800	4.126300	-1.049900
H	-3.323900	5.137000	-1.129200
C	-5.038100	3.880500	-1.335100
H	-5.689200	4.692800	-1.632800
C	-5.530900	2.589800	-1.243300
H	-6.571400	2.398300	-1.478500
C	-4.707300	1.530000	-0.876700
C	-1.402400	3.413500	-0.324100
H	-1.022100	2.614500	0.313600
C	-0.557500	3.449600	-1.602100
H	-0.655100	2.531300	-2.185900
H	0.497500	3.585600	-1.351500
H	-0.876500	4.276500	-2.242500
C	-1.218600	4.716400	0.452600
H	-1.453400	5.591200	-0.157100
H	-0.176600	4.795600	0.765100
H	-1.850400	4.740300	1.341700
C	-5.266100	0.120100	-0.863100
H	-4.421500	-0.564200	-0.785400
C	-6.194300	-0.120200	0.331100
H	-7.060600	0.543900	0.280400
H	-5.696400	0.060000	1.285000
H	-6.557500	-1.150500	0.327800
C	-5.996600	-0.216000	-2.165600
H	-6.913100	0.367200	-2.272000
H	-6.274100	-1.271700	-2.175100
H	-5.366300	-0.017600	-3.033300
C	-2.793900	-1.416500	0.916700
C	-1.936000	-1.904100	0.026900
C	-1.750600	-3.329400	-0.311200
C	-1.477200	-4.839300	-2.081500
H	-1.427700	-4.790900	-3.164900
H	-2.307400	-5.468500	-1.763500
H	-0.548500	-5.234700	-1.672600

C	-3.767500	-2.179900	1.739300
C	-5.280900	-3.954500	1.818700
H	-6.071600	-3.329100	2.231000
H	-4.756800	-4.456600	2.630300
H	-5.687700	-4.678700	1.120200

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C	-1.253300	1.477400	3.753600
H	-2.179300	1.736000	4.253300
C	-1.289300	0.955300	2.439400
C	-2.450200	0.733900	1.680300
H	-3.462800	0.936900	2.009000
N	-2.231200	0.248000	0.469900
C	-0.089400	0.609900	1.755100
C	-0.047500	1.655100	4.367900
H	0.003400	2.062600	5.369000
C	1.149000	1.302900	3.699800
H	2.096300	1.444200	4.208600
C	1.146000	0.774800	2.433700
C	2.437200	0.317100	1.802800
H	2.626000	-0.722800	2.082500
N	2.369200	0.379500	0.344600
C	3.465900	-0.210900	-0.347400
C	3.536300	-1.608200	-0.442400
C	4.453300	0.601800	-0.936200
C	4.615100	-2.175000	-1.115900
C	5.500700	-0.008200	-1.617100
C	5.591000	-1.389200	-1.701700
H	4.680400	-3.254000	-1.194300
H	6.268400	0.599900	-2.076700
H	6.419500	-1.848900	-2.225200
C	-3.302900	0.007100	-0.447600
C	-3.762300	1.067400	-1.237900
C	-3.836600	-1.283500	-0.541800
C	-4.789000	0.805600	-2.140200
C	-4.857400	-1.495500	-1.464200
C	-5.332100	-0.463200	-2.256300
H	-5.163500	1.607900	-2.764500
H	-5.284300	-2.486100	-1.564700
H	-6.126400	-0.648400	-2.968200
C	4.345000	2.114500	-0.865800
H	3.955500	2.374700	0.123700
C	3.361100	2.629500	-1.925200
H	2.381000	2.152800	-1.854600
H	3.224800	3.708600	-1.834500
H	3.754300	2.416200	-2.921500
C	5.682200	2.835700	-1.011300
H	6.425400	2.444900	-0.315300
H	6.078600	2.742800	-2.023900
H	5.549300	3.899700	-0.811200

C	2.457500	-2.517500	0.115600
H	1.711800	-1.905100	0.619500
C	3.021400	-3.511300	1.132700
H	2.217100	-4.111800	1.561100
H	3.733500	-4.193200	0.663300
H	3.538400	-2.999600	1.946800
C	1.730800	-3.250100	-1.014400
H	0.924500	-3.864300	-0.608400
H	1.296900	-2.539700	-1.719900
H	2.413200	-3.903100	-1.562600
C	-3.324900	-2.433900	0.302100
H	-2.633000	-2.032100	1.043200
C	-2.550600	-3.427600	-0.566700
H	-1.716000	-2.936400	-1.069500
H	-2.154600	-4.239800	0.045900
H	-3.202900	-3.861300	-1.328100
C	-4.458100	-3.134200	1.053500
H	-5.027700	-2.427200	1.658300
H	-5.149600	-3.623900	0.365100
H	-4.050800	-3.900800	1.714300
C	-3.178500	2.463400	-1.143100
H	-2.389500	2.455400	-0.390100
C	-2.542300	2.882500	-2.469900
H	-2.086700	3.869500	-2.373300
H	-1.769500	2.174400	-2.772400
H	-3.289000	2.933200	-3.265200
C	-4.238200	3.474400	-0.701300
H	-5.038500	3.553100	-1.440000
H	-4.686100	3.185200	0.250700
H	-3.791500	4.463200	-0.584600
As	-0.415500	-0.021200	0.007600
H	3.276000	0.903000	2.200600
H	2.236100	1.340600	0.060800

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C	1.217300	-0.952100	3.857200
H	2.156100	-1.148100	4.362400
C	1.220400	-0.618000	2.486200
C	2.406400	-0.514800	1.711300
H	3.394600	-0.694100	2.127800
N	2.276900	-0.192200	0.449800
C	0.008800	-0.358900	1.799300
C	0.027200	-1.028500	4.530900
H	0.007600	-1.291500	5.580300
C	-1.181200	-0.759000	3.857300
H	-2.116100	-0.814500	4.404800
C	-1.199600	-0.415800	2.524700
C	-2.498100	-0.039800	1.852800
H	-2.688500	1.026300	1.999400
N	-2.434100	-0.290500	0.408100

C	-3.574800	0.145000	-0.337600
C	-3.733100	1.509200	-0.615300
C	-4.512900	-0.800100	-0.795700
C	-4.850000	1.911900	-1.344000
C	-5.601100	-0.352500	-1.535200
C	-5.777800	0.996200	-1.804200
H	-4.984200	2.964100	-1.565400
H	-6.330700	-1.063100	-1.899400
H	-6.636100	1.327500	-2.374400
C	3.421100	-0.079000	-0.397600
C	3.891200	-1.219700	-1.061900
C	4.014100	1.178800	-0.569400
C	4.979900	-1.072000	-1.916200
C	5.100600	1.273400	-1.434100
C	5.582000	0.161100	-2.104100
H	5.360300	-1.938500	-2.444000
H	5.575500	2.235800	-1.584500
H	6.426700	0.254800	-2.774600
C	-4.308500	-2.281600	-0.531400
H	-3.903700	-2.390500	0.480200
C	-3.295300	-2.863400	-1.527100
H	-2.345200	-2.324000	-1.525700
H	-3.092800	-3.912500	-1.304900
H	-3.702700	-2.798300	-2.538200
C	-5.597100	-3.098900	-0.571200
H	-6.364900	-2.669300	0.073400
H	-5.996400	-3.164900	-1.584600
H	-5.395500	-4.116600	-0.234800
C	-2.720200	2.555600	-0.190700
H	-1.913300	2.061300	0.348000
C	-3.342300	3.596300	0.742300
H	-2.583000	4.301600	1.083900
H	-4.121300	4.164100	0.229600
H	-3.795600	3.128100	1.617900
C	-2.085800	3.228600	-1.409300
H	-1.316600	3.934700	-1.090400
H	-1.619700	2.490100	-2.063300
H	-2.831500	3.776300	-1.989100
C	3.512900	2.416200	0.149300
H	2.680900	2.126000	0.791400
C	2.983900	3.450400	-0.846100
H	2.178700	3.029800	-1.450900
H	2.595300	4.321400	-0.315300
H	3.776000	3.789300	-1.517200
C	4.602400	3.018500	1.038500
H	4.972400	2.286900	1.758400
H	5.450500	3.364100	0.444000
H	4.208900	3.874700	1.589000
C	3.252700	-2.584200	-0.886600
H	2.450700	-2.496900	-0.153300

C	2.626200	-3.065000	-2.196900
H	2.138900	-4.030700	-2.050800
H	1.879600	-2.354300	-2.554500
H	3.385700	-3.184100	-2.972600
C	4.261800	-3.604900	-0.356500
H	5.070200	-3.767200	-1.072000
H	4.704700	-3.269400	0.582500
H	3.772100	-4.564400	-0.182800
H	-3.335300	-0.576400	2.315300
H	-2.291700	-1.283100	0.270700
Sb	0.260600	0.085900	-0.226200

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7-As

H	-2.597100	0.105900	0.793500
O	0.953900	4.012500	0.820400
N	-2.593600	-0.708600	0.190300
C	0.053900	-0.841300	1.330000
N	2.244900	-0.395400	0.073800
O	2.341300	3.132400	2.342900
C	-1.049400	-1.460600	1.881100
O	-1.619600	2.554700	-0.330500
C	-1.104100	-1.571000	3.273900
H	-1.955000	-2.056800	3.737600
C	-0.088600	-1.053100	4.065100
H	-0.148400	-1.151700	5.141500
O	-0.146400	2.858900	-1.991300
C	0.995000	-0.382100	3.494100
H	1.765300	0.055100	4.118000
C	1.056600	-0.286400	2.118000
C	-2.182800	-1.879300	0.985600
H	-1.867500	-2.668100	0.294300
H	-3.008700	-2.285000	1.582200
C	-3.893800	-1.335900	-1.770800
C	-3.866300	-0.865300	-0.450400
C	-5.128700	-1.522100	-2.384000
H	-5.174200	-1.892000	-3.399600
C	-6.307000	-1.228900	-1.715300
H	-7.260200	-1.375200	-2.207700
C	-6.266300	-0.747800	-0.417400
H	-7.193600	-0.523300	0.093000
C	-5.052200	-0.569800	0.241000
C	-2.596700	-1.538700	-2.528600
H	-1.859500	-1.942400	-1.832500
C	-2.705900	-2.506600	-3.702300
H	-3.321000	-2.095800	-4.505300
H	-3.135600	-3.462400	-3.398000
H	-1.714300	-2.692700	-4.117000
C	-2.083500	-0.176100	-3.005300
H	-2.784700	0.257500	-3.722700
H	-1.108900	-0.269700	-3.488400

H	-1.988500	0.511200	-2.162800
C	-6.249700	-0.344100	2.479600
H	-7.120200	0.210000	2.124200
H	-6.086500	-0.059100	3.519800
H	-6.486400	-1.408400	2.447600
C	-5.005300	-0.022000	1.656100
H	-4.155300	-0.482100	2.167900
C	-4.770700	1.493100	1.631600
H	-5.598900	1.988200	1.119300
H	-3.850000	1.754400	1.106600
H	-4.706000	1.890900	2.645900
C	2.082400	0.445200	1.251800
H	3.018200	0.683000	1.754000
C	3.479000	-0.853700	-0.446800
C	4.101600	-0.166900	-1.507000
C	5.307000	-0.655600	-2.000800
H	5.799000	-0.146300	-2.819400
C	5.896000	-1.785200	-1.454000
H	6.838400	-2.147200	-1.845800
C	5.276800	-2.454300	-0.412600
H	5.741900	-3.340400	0.000800
C	4.058600	-2.013600	0.097900
C	3.502600	1.115300	-2.047100
H	2.417800	1.047200	-1.954000
C	3.961300	2.299700	-1.189300
H	5.029200	2.477000	-1.338900
H	3.807300	2.109100	-0.126200
H	3.416000	3.205600	-1.462700
C	3.811600	1.377600	-3.518200
H	3.550500	0.519700	-4.139600
H	4.867200	1.606000	-3.676500
H	3.235900	2.237900	-3.862200
C	3.395200	-2.759700	1.237200
H	2.336000	-2.498600	1.226200
C	3.973400	-2.307200	2.581300
H	3.465400	-2.811200	3.406000
H	3.864500	-1.231400	2.722700
H	5.038400	-2.546600	2.633100
C	3.503000	-4.278300	1.102600
H	3.163900	-4.616600	0.122600
H	2.888100	-4.760100	1.864400
H	4.527800	-4.625300	1.246200
C	0.436200	1.443400	-0.190500
C	1.336900	1.700400	0.748800
C	1.607500	3.003300	1.395800
C	1.179600	5.302500	1.390700
H	2.237100	5.556400	1.336100
H	0.859700	5.314600	2.431400
H	0.588700	5.994000	0.798700
C	-0.438800	2.376300	-0.930000

C	-2.538400	3.388800	-1.044600
H	-2.757700	2.953100	-2.018700
H	-2.113600	4.382100	-1.179900
H	-3.435700	3.433600	-0.435600
As	0.517000	-0.545000	-0.569800

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7-Sb

H	-2.527500	0.066200	0.747300
O	0.867200	3.970400	0.859000
N	-2.626600	-0.770000	0.181100
C	-0.007200	-0.958800	1.297700
N	2.290000	-0.423500	0.025800
O	2.150300	3.010800	2.422100
C	-1.113600	-1.534800	1.892100
O	-1.681500	2.578500	-0.374700
C	-1.167500	-1.577900	3.286800
H	-2.022000	-2.029200	3.778400
C	-0.142600	-1.026100	4.044400
H	-0.195300	-1.068900	5.124900
O	-0.193200	2.984300	-2.000100
C	0.931900	-0.380000	3.432600
H	1.697800	0.101700	4.028900
C	0.992600	-0.351800	2.049900
C	-2.268700	-1.938500	1.015100
H	-1.996500	-2.763700	0.347900
H	-3.113100	-2.279900	1.623800
C	-4.109800	-1.296000	-1.682600
C	-3.951700	-0.835600	-0.368600
C	-5.395100	-1.379200	-2.208300
H	-5.540300	-1.737600	-3.218800
C	-6.496400	-1.001800	-1.456600
H	-7.490300	-1.071100	-1.880400
C	-6.326700	-0.537700	-0.162600
H	-7.195600	-0.246700	0.412900
C	-5.058900	-0.455400	0.407100
C	-2.892000	-1.600700	-2.531000
H	-2.132600	-2.034900	-1.877600
C	-3.151600	-2.593500	-3.659600
H	-3.802000	-2.169400	-4.426900
H	-3.613900	-3.509800	-3.289300
H	-2.209400	-2.855600	-4.142700
C	-2.337000	-0.287600	-3.093600
H	-3.066400	0.164900	-3.769600
H	-1.413100	-0.457300	-3.650200
H	-2.136500	0.427000	-2.291500
C	-6.066900	-0.171100	2.729200
H	-6.934600	0.424400	2.440400
H	-5.811000	0.104100	3.753100
H	-6.356300	-1.223000	2.717300
C	-4.875200	0.092200	1.811700

H	-4.010000	-0.400900	2.262100
C	-4.574900	1.594800	1.757600
H	-5.409300	2.122700	1.289600
H	-3.674300	1.809900	1.179100
H	-4.434200	1.995900	2.762800
C	2.012100	0.403400	1.192300
H	2.911800	0.679300	1.741100
C	3.601800	-0.759000	-0.383500
C	4.279500	0.027700	-1.336700
C	5.561400	-0.347400	-1.726500
H	6.093800	0.244200	-2.460200
C	6.174700	-1.465600	-1.184000
H	7.175300	-1.739200	-1.494700
C	5.505500	-2.233000	-0.246300
H	5.992000	-3.105700	0.171400
C	4.215900	-1.903100	0.161200
C	3.654000	1.299300	-1.871900
H	2.570500	1.179600	-1.845100
C	4.002700	2.474400	-0.951400
H	5.068500	2.703900	-1.027100
H	3.792800	2.242700	0.094100
H	3.433700	3.364100	-1.230800
C	4.040200	1.626000	-3.312200
H	3.858800	0.779700	-3.976600
H	5.091800	1.906400	-3.395800
H	3.448300	2.471900	-3.665000
C	3.511500	-2.742700	1.206800
H	2.443100	-2.538100	1.123700
C	3.954600	-2.320700	2.610800
H	3.410800	-2.884200	3.371800
H	3.774200	-1.258600	2.781700
H	5.023700	-2.505700	2.741100
C	3.721200	-4.243800	1.012900
H	3.476300	-4.551500	-0.004800
H	3.084300	-4.799800	1.702800
H	4.752900	-4.537500	1.215800
C	0.370400	1.462200	-0.279000
C	1.249000	1.656600	0.697000
C	1.480100	2.929500	1.423600
C	1.052600	5.226800	1.511800
H	2.110700	5.482500	1.539200
H	0.666300	5.182700	2.528900
H	0.499500	5.950700	0.921800
C	-0.488100	2.441200	-0.968000
C	-2.596300	3.446300	-1.050800
H	-2.812100	3.060300	-2.046300
H	-2.172000	4.445400	-1.135900
H	-3.496800	3.461100	-0.444700
Sb	0.444200	-0.686900	-0.788800

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8-As

As	0.474400	2.061700	0.229000
H	-4.296400	0.051500	0.613100
O	-0.668500	4.675700	-0.552300
N	-3.441100	-0.470200	0.488100
C	0.217600	0.223100	0.667200
O	-2.489100	4.521900	0.735900
H	4.031400	-0.948600	1.828000
N	3.849900	-0.898800	0.836500
C	-1.051900	-0.357700	0.895400
O	-3.674200	2.935300	-1.230600
C	-1.111800	-1.642400	1.489500
H	-2.067000	-2.054700	1.775700
C	0.025500	-2.362300	1.723800
H	-0.040800	-3.341300	2.180500
O	-4.770700	1.966500	0.453600
C	1.277700	-1.838700	1.372000
H	2.172200	-2.431300	1.508500
C	1.387800	-0.560600	0.881300
C	-2.299000	0.292800	0.542000
C	-3.598400	-1.794100	-0.004100
C	-2.953300	-2.238300	-1.166800
C	-3.151600	-3.563200	-1.554400
H	-2.650600	-3.928900	-2.442700
C	-3.984800	-4.410600	-0.849600
H	-4.125500	-5.432500	-1.177300
C	-4.646400	-3.940900	0.275700
H	-5.301400	-4.605100	0.823700
C	-4.460300	-2.639800	0.721000
C	-2.093400	-1.357700	-2.057500
H	-2.057100	-0.350300	-1.648200
C	-0.655000	-1.875000	-2.148300
H	-0.210400	-2.004800	-1.160100
H	-0.039800	-1.171600	-2.712800
H	-0.622200	-2.837900	-2.663100
C	-2.713300	-1.235300	-3.453000
H	-2.759400	-2.205000	-3.951700
H	-2.112700	-0.566700	-4.072200
H	-3.726900	-0.836000	-3.396700
C	-5.173400	-2.118600	1.953200
H	-4.497000	-1.411500	2.442000
C	-6.445700	-1.358200	1.557100
H	-7.148200	-2.041800	1.075200
H	-6.250900	-0.540700	0.860600
H	-6.928200	-0.935000	2.439500
C	-1.294500	2.529600	0.191600
C	-2.392800	1.656900	0.260000
C	-3.735400	2.199100	-0.123200
C	-4.876100	3.624700	-1.578200
H	-5.679800	2.914300	-1.763500

H	-4.645100	4.186800	-2.477500
H	-5.159600	4.293200	-0.766100
C	-1.575100	3.996200	0.152600
C	-0.822200	6.095000	-0.546400
H	-1.784800	6.369500	-0.975600
H	-0.008600	6.482900	-1.151200
H	-0.761500	6.477200	0.471500
C	2.751600	0.023400	0.575200
H	2.791600	0.307100	-0.478400
H	2.879100	0.959500	1.136200
C	5.040200	-0.659200	0.099300
C	6.186200	-0.138000	0.728800
C	7.331600	0.064300	-0.032500
H	8.220900	0.466500	0.434200
C	7.349000	-0.216400	-1.390000
H	8.245300	-0.037900	-1.970000
C	6.215100	-0.728700	-1.995900
H	6.235900	-0.961400	-3.054300
C	5.053700	-0.971800	-1.269100
C	6.176700	0.157000	2.217700
H	5.192300	0.565400	2.468400
C	6.386100	-1.134400	3.019500
H	5.666600	-1.911700	2.755400
H	6.308100	-0.943100	4.091300
H	7.381900	-1.533200	2.814400
C	7.205400	1.199200	2.647700
H	7.042100	1.467600	3.692200
H	7.136200	2.105000	2.044300
H	8.222000	0.810400	2.567400
C	3.864700	-1.614000	-1.961900
H	3.072500	-1.753900	-1.225300
C	4.232800	-3.003400	-2.489100
H	4.608900	-3.638300	-1.686200
H	5.003700	-2.940100	-3.259900
H	3.357000	-3.484000	-2.929000
C	3.326200	-0.740500	-3.096600
H	2.470100	-1.221300	-3.572800
H	4.089700	-0.585800	-3.861900
H	3.011800	0.242300	-2.739800
C	-5.515600	-3.205500	2.968100
H	-5.889300	-2.747200	3.884600
H	-4.642400	-3.809700	3.219000
H	-6.297100	-3.871500	2.597400

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8-Sb

H	4.284300	-0.270100	-0.648100
O	1.201900	4.742100	0.603600
N	3.379600	-0.697100	-0.517200
C	-0.224300	0.256300	-0.677900
O	3.113700	4.342600	-0.484800

H	-4.130000	-0.524400	-1.915500
N	-3.898100	-0.704700	-0.950500
C	1.024000	-0.349000	-0.960400
O	3.986600	2.483300	1.385100
C	1.031500	-1.580600	-1.661900
H	1.971000	-2.006600	-1.979600
C	-0.131900	-2.232700	-1.963100
H	-0.100800	-3.167500	-2.507600
O	4.967300	1.584800	-0.406600
C	-1.361500	-1.698600	-1.560300
H	-2.280900	-2.237600	-1.745000
C	-1.417200	-0.468200	-0.949100
C	2.318300	0.185600	-0.552400
C	3.399700	-2.037200	-0.052700
C	2.683600	-2.450400	1.081000
C	2.757400	-3.794700	1.445100
H	2.200000	-4.132000	2.311000
C	3.537600	-4.697000	0.748400
H	3.582300	-5.733100	1.058300
C	4.269600	-4.262800	-0.347000
H	4.882900	-4.969400	-0.890200
C	4.207400	-2.943100	-0.770300
C	1.870300	-1.521700	1.965200
H	1.940400	-0.504900	1.585000
C	0.389400	-1.913200	1.982500
H	-0.013600	-2.015500	0.973600
H	-0.192600	-1.154200	2.509800
H	0.247300	-2.865200	2.500000
C	2.434500	-1.490400	3.388400
H	2.363700	-2.470800	3.863100
H	1.871700	-0.781200	3.998100
H	3.482800	-1.188600	3.388500
C	5.003800	-2.465800	-1.968700
H	4.411000	-1.692300	-2.465500
C	6.326100	-1.830800	-1.518100
H	6.949700	-2.586300	-1.034900
H	6.184100	-1.016400	-0.805400
H	6.871000	-1.431800	-2.375200
C	1.600200	2.534000	-0.099900
C	2.563800	1.515500	-0.208600
C	3.965800	1.865300	0.206000
C	5.255800	3.001900	1.784600
H	5.985900	2.198900	1.869100
H	5.092800	3.474200	2.748300
H	5.597700	3.730500	1.050000
C	2.081100	3.935800	-0.012300
C	1.543000	6.127200	0.622700
H	2.489500	6.274400	1.140400
H	0.736000	6.624700	1.151500
H	1.628800	6.509500	-0.393600

C -2.760700 0.109100 -0.542200
H -2.788100 0.207200 0.546500
H -2.856300 1.130000 -0.937200
C -5.044100 -0.670000 -0.114900
C -6.227400 -0.036500 -0.540500
C -7.335300 -0.059600 0.299600
H -8.253900 0.420400 -0.010900
C -7.280000 -0.668800 1.543600
H -8.149000 -0.666500 2.188900
C -6.108500 -1.281700 1.951400
H -6.071600 -1.770600 2.918200
C -4.982300 -1.307300 1.134100
C -6.296600 0.622500 -1.906000
H -5.325100 1.090100 -2.096300
C -6.551600 -0.426200 -2.996200
H -5.823000 -1.238600 -2.970800
H -6.524900 0.029500 -3.987600
H -7.537900 -0.871900 -2.850200
C -7.341600 1.730700 -2.003900
H -7.238800 2.249300 -2.958000
H -7.228700 2.460600 -1.201500
H -8.354900 1.328000 -1.961100
C -3.754300 -2.074000 1.593600
H -2.977800 -1.979200 0.834100
C -4.072300 -3.566200 1.719600
H -4.452900 -3.963300 0.777600
H -4.826400 -3.741700 2.489500
H -3.174100 -4.123700 1.992300
C -3.203800 -1.529700 2.912600
H -2.322300 -2.095900 3.217100
H -3.945700 -1.611200 3.709500
H -2.922400 -0.477800 2.827100
C 5.282300 -3.561600 -2.994200
H 5.717500 -3.122000 -3.892400
H 4.369700 -4.088200 -3.277200
H 5.995800 -4.294900 -2.613600
Sb -0.404000 2.271800 -0.088300
92
9-As
As 1.169800 -0.099700 0.592400
H -3.463100 -1.015500 1.318500
O 1.796500 -2.892800 -1.189600
N -3.108500 -0.405900 0.586200
C 0.050700 0.383100 -0.904500
O -0.330200 -2.645000 -1.835900
N 2.585100 0.277900 -0.547000
C -1.293400 0.055800 -0.963200
C -1.989500 0.301800 -2.138900
H -3.037900 0.046700 -2.223300
O -0.752500 -3.263200 2.493900

C	-1.316200	0.840500	-3.233000
H	-1.861100	1.033200	-4.147800
O	-2.750700	-2.284300	2.391900
C	0.051600	1.073200	-3.188000
H	0.572700	1.420300	-4.072700
C	0.751900	0.818100	-2.011400
C	-1.853700	-0.690100	0.196600
C	-3.498900	2.011100	0.347900
C	-3.920000	0.688200	0.169700
C	-4.350900	3.027500	-0.081700
H	-4.043400	4.059000	0.040700
C	-5.581900	2.746000	-0.643700
H	-6.228000	3.552400	-0.966400
C	-5.990700	1.428200	-0.789700
H	-6.955300	1.218400	-1.232600
C	-5.170800	0.380200	-0.392700
C	-2.193500	2.390500	1.021700
H	-1.629800	1.484500	1.239800
C	-1.329000	3.282900	0.126500
H	-0.341600	3.417100	0.575400
H	-1.777900	4.271900	0.012100
H	-1.198800	2.850300	-0.866700
C	-2.463500	3.076300	2.364100
H	-3.054300	2.435900	3.020100
H	-3.009500	4.010800	2.220300
H	-1.520900	3.307700	2.864100
C	-5.603200	-1.064900	-0.541600
H	-4.705500	-1.651200	-0.756100
C	-6.587600	-1.290600	-1.685700
H	-6.218600	-0.868500	-2.621700
H	-7.562200	-0.847800	-1.471100
H	-6.742100	-2.360500	-1.830600
C	-6.201100	-1.582300	0.772400
H	-6.481000	-2.632500	0.675700
H	-7.096500	-1.009400	1.023800
H	-5.505500	-1.498200	1.608500
C	-1.068700	-1.659100	0.813600
C	0.347700	-1.961700	0.380500
H	0.838100	-2.613600	1.095700
C	0.518100	-2.532800	-0.990100
C	2.111900	-3.378100	-2.490000
H	3.170100	-3.626600	-2.465100
H	1.919600	-2.608700	-3.238200
H	1.519100	-4.260700	-2.726300
C	-1.618100	-2.394900	1.942600
C	-1.247400	-4.014800	3.598300
H	-0.426400	-4.653100	3.910800
H	-2.104800	-4.615000	3.297800
H	-1.544800	-3.351300	4.409100
C	2.248800	0.849800	-1.853400

H	2.719200	0.282800	-2.667700
H	2.635200	1.874700	-1.922200
C	3.838300	0.687400	0.002900
C	3.981500	1.973500	0.553300
C	5.219000	2.340000	1.076300
H	5.343100	3.325000	1.511400
C	6.291500	1.465500	1.056000
H	7.245500	1.767900	1.469200
C	6.142200	0.203500	0.502900
H	6.987300	-0.472900	0.488500
C	4.924500	-0.202300	-0.033300
C	2.838700	2.971600	0.613000
H	1.966200	2.537700	0.119900
C	2.446300	3.269000	2.062600
H	2.165800	2.356000	2.589300
H	1.601700	3.960400	2.095500
H	3.277400	3.730300	2.600200
C	3.181100	4.267100	-0.126100
H	4.004800	4.790500	0.362900
H	2.317800	4.935100	-0.134400
H	3.474700	4.070800	-1.158400
C	4.749700	-1.595800	-0.598700
H	3.917200	-1.552500	-1.302100
C	4.355300	-2.562100	0.520800
H	4.175800	-3.562700	0.122900
H	3.443100	-2.232300	1.021400
H	5.153200	-2.620100	1.265500
C	5.983400	-2.110900	-1.336600
H	6.812000	-2.305800	-0.653100
H	6.325900	-1.400300	-2.090500
H	5.750900	-3.053900	-1.835000

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9-Sb

H	3.667500	-0.906000	-1.263100
O	-1.543700	-2.967300	1.132800
N	3.264200	-0.319800	-0.537200
C	0.040300	0.413600	0.837600
O	0.573200	-2.651000	1.782800
N	-2.605200	0.348600	0.518000
C	1.380100	0.068800	0.945200
C	2.040700	0.283000	2.147300
H	3.080600	0.005800	2.262500
O	1.069100	-3.150100	-2.651400
C	1.340700	0.812900	3.227700
H	1.856000	0.980800	4.164400
O	3.034500	-2.127300	-2.430800
C	-0.019600	1.065700	3.136800
H	-0.567100	1.407000	4.008300
C	-0.688400	0.840300	1.933900
C	2.005700	-0.651800	-0.200200

C	3.613000	2.099700	-0.266100
C	4.036200	0.781600	-0.066100
C	4.428700	3.124800	0.210400
H	4.118800	4.153300	0.070200
C	5.627500	2.854500	0.843400
H	6.246700	3.666800	1.202200
C	6.037800	1.540400	1.016500
H	6.974900	1.338700	1.518100
C	5.252800	0.485000	0.571800
C	2.339600	2.462200	-1.005500
H	1.803800	1.546200	-1.251600
C	1.419200	3.336000	-0.148800
H	0.449700	3.455500	-0.638900
H	1.845700	4.332000	-0.012000
H	1.255100	2.895700	0.836200
C	2.666500	3.156200	-2.330700
H	3.289900	2.522300	-2.962400
H	3.200600	4.092400	-2.157200
H	1.747300	3.387000	-2.872400
C	5.684400	-0.956500	0.755500
H	4.777700	-1.548500	0.909500
C	6.587500	-1.169800	1.967100
H	6.153100	-0.742100	2.872000
H	7.573000	-0.724500	1.817600
H	6.735300	-2.237900	2.130700
C	6.375500	-1.475800	-0.510700
H	6.658500	-2.522400	-0.386900
H	7.280700	-0.896100	-0.705100
H	5.737000	-1.404700	-1.392300
C	1.286900	-1.644200	-0.867200
C	-0.100400	-2.071700	-0.460400
H	-0.511200	-2.794600	-1.156600
C	-0.268900	-2.585200	0.924900
C	-1.846500	-3.431000	2.443400
H	-2.900400	-3.697900	2.427500
H	-1.665900	-2.643800	3.175900
H	-1.238400	-4.298700	2.696000
C	1.894600	-2.296300	-2.020200
C	1.618100	-3.820000	-3.782600
H	0.827300	-4.463700	-4.156100
H	2.485400	-4.410800	-3.491900
H	1.917000	-3.101000	-4.544100
C	-2.188100	0.926500	1.792100
H	-2.655500	0.399000	2.635800
H	-2.523700	1.971300	1.862900
C	-3.941700	0.642000	0.127000
C	-4.259100	1.898400	-0.422400
C	-5.574700	2.152800	-0.800300
H	-5.828100	3.114400	-1.231700
C	-6.562500	1.195800	-0.642600

H -7.579800 1.409700 -0.945600
C -6.244300 -0.036300 -0.094600
H -7.021800 -0.780100 0.027100
C -4.943900 -0.329400 0.303100
C -3.211600 2.974800 -0.641500
H -2.263900 2.622200 -0.229800
C -2.997600 3.234700 -2.135000
H -2.713500 2.320200 -2.658400
H -2.210900 3.977000 -2.285100
H -3.911800 3.614700 -2.595900
C -3.572400 4.273000 0.083000
H -4.485500 4.709300 -0.326500
H -2.772200 5.006300 -0.031700
H -3.732600 4.101000 1.148500
C -4.599900 -1.692400 0.867300
H -3.681100 -1.579000 1.443900
C -4.309300 -2.669800 -0.274600
H -4.028600 -3.650900 0.113500
H -3.488400 -2.315800 -0.901800
H -5.194100 -2.783900 -0.905900
C -5.682400 -2.256900 1.785100
H -6.586900 -2.516900 1.232300
H -5.954300 -1.545800 2.566500
H -5.326100 -3.171600 2.263100
Sb -1.147100 -0.128300 -0.829600
92
10_Sb
O -0.031100 -2.905200 1.201300
N -2.556300 0.172400 -0.621900
C -0.310800 -1.360300 -1.484700
O -2.062700 -2.037200 1.584500
N 2.128400 -0.597500 -0.696600
C -1.615400 -1.625200 -1.900800
C -1.878800 -2.741000 -2.690900
H -2.891400 -2.942600 -3.021900
O 1.722900 1.413400 1.885000
C -0.841700 -3.598800 -3.039800
H -1.046000 -4.470100 -3.648600
O 1.219800 1.591400 4.059300
C 0.451900 -3.344400 -2.607800
H 1.255200 -4.021200 -2.877700
C 0.724400 -2.216100 -1.833500
C -2.717000 -0.747600 -1.481200
C -3.602800 2.327900 -0.273200
C -3.688800 0.923800 -0.209200
C -4.706400 3.081100 0.101400
H -4.660400 4.160900 0.042000
C -5.867000 2.473200 0.556200
H -6.720800 3.074000 0.842000
C -5.919300 1.096800 0.658400

H	-6.817600	0.626800	1.040500
C	-4.842400	0.291000	0.288700
C	-2.314500	3.013500	-0.681000
H	-1.739600	2.317100	-1.291500
C	-2.526700	4.274900	-1.516300
H	-1.565400	4.641800	-1.879800
H	-2.979400	5.077500	-0.931900
H	-3.167000	4.077900	-2.377300
C	-1.499600	3.335200	0.576500
H	-1.367100	2.449400	1.201800
H	-2.020900	4.087000	1.174100
H	-0.512900	3.723000	0.312600
C	-4.968200	-1.207900	0.507800
H	-4.016200	-1.683800	0.284400
C	-6.043700	-1.818500	-0.393800
H	-5.836300	-1.641200	-1.450900
H	-7.024000	-1.389100	-0.176300
H	-6.106700	-2.896300	-0.232500
C	-5.259000	-1.520900	1.977600
H	-5.260800	-2.601200	2.132800
H	-6.232600	-1.135000	2.286000
H	-4.492300	-1.087900	2.619400
C	0.236300	-0.162900	2.787700
C	-0.123300	-0.627200	1.595100
C	-0.870800	-1.903000	1.490700
C	-0.648900	-4.132100	0.808200
H	0.165300	-4.817500	0.591800
H	-1.253600	-3.965800	-0.084900
H	-1.275800	-4.519300	1.609500
C	1.079700	1.039600	3.000500
C	2.644200	2.500000	1.999100
H	3.134600	2.570100	1.030700
H	3.375000	2.282900	2.777100
H	2.112000	3.418300	2.242900
C	2.112500	-1.903500	-1.325900
H	2.410400	-2.708000	-0.636000
H	2.824700	-1.928000	-2.162300
C	3.377900	0.009800	-0.420600
C	3.858900	1.028500	-1.266100
C	5.049000	1.676000	-0.938600
H	5.414900	2.471700	-1.577200
C	5.773900	1.317600	0.183900
H	6.697000	1.830200	0.423600
C	5.313200	0.292600	0.996600
H	5.887500	0.009500	1.871100
C	4.122200	-0.368000	0.716300
C	3.121500	1.452600	-2.522100
H	2.287800	0.763900	-2.667700
C	2.559100	2.869600	-2.379300
H	1.901800	2.951500	-1.511100

H 1.988600 3.149100 -3.267200
H 3.368900 3.592800 -2.257100
C 4.015600 1.356300 -3.760400
H 4.849400 2.058400 -3.702400
H 3.443000 1.595100 -4.658400
H 4.427800 0.352500 -3.870800
C 3.653800 -1.490300 1.619400
H 2.604000 -1.682800 1.388300
C 3.751900 -1.139900 3.105200
H 3.233500 -1.892800 3.701700
H 3.310900 -0.167400 3.325100
H 4.790600 -1.114600 3.441400
C 4.457200 -2.766300 1.341700
H 5.507500 -2.611300 1.600600
H 4.415200 -3.049200 0.289300
H 4.078800 -3.597400 1.940300
Sb 0.335300 0.325300 -0.348800
H -0.046600 -0.655400 3.713300
H -3.695500 -0.935300 -1.933800
92
11_As (isomer 1)
O -5.296100 -0.193700 -0.387700
N -1.356600 -0.495100 0.015500
C 0.520100 0.715300 -1.151800
O -3.956100 -1.004100 -1.988900
N 3.209200 0.365500 -0.208700
C -0.782800 1.207700 -1.427900
O -3.427500 4.397200 -0.703900
C -0.961100 2.266800 -2.351200
H -1.958000 2.621200 -2.585300
C 0.129000 2.822200 -2.955000
H 0.004500 3.631000 -3.663000
O -1.951600 3.297500 0.568300
C 1.429600 2.333300 -2.681300
H 2.279700 2.782200 -3.182700
C 1.633700 1.288600 -1.819700
C -1.800500 0.527300 -0.726200
C -2.725100 -0.725600 2.028200
C -2.241000 -1.279200 0.834600
C -3.601000 -1.491300 2.793000
H -3.984500 -1.087800 3.721800
C -3.979600 -2.759700 2.390200
H -4.662800 -3.340500 2.997200
C -3.472600 -3.293300 1.216500
H -3.763400 -4.292200 0.917900
C -2.591900 -2.572800 0.414700
C -2.278400 0.631100 2.533800
H -1.757200 1.155600 1.734500
C -3.454800 1.508300 2.963100
H -3.098500 2.515600 3.183200

H	-3.936300	1.120300	3.862900
H	-4.208700	1.573300	2.176200
C	-1.291200	0.450800	3.691100
H	-0.427700	-0.139300	3.379900
H	-1.770800	-0.060100	4.529400
H	-0.936600	1.422300	4.039700
C	-2.015100	-3.213100	-0.833300
H	-1.637600	-2.418000	-1.478000
C	-3.049700	-4.008300	-1.631300
H	-3.927200	-3.404800	-1.857300
H	-3.362600	-4.906700	-1.095800
H	-2.607700	-4.333100	-2.574600
C	-0.848900	-4.133100	-0.451700
H	-0.401100	-4.565200	-1.348900
H	-1.208700	-4.950300	0.178300
H	-0.071700	-3.599400	0.095000
C	-3.227200	0.882600	-0.736200
C	-3.721500	2.105000	-0.531600
H	-4.784400	2.279600	-0.645100
C	-2.913000	3.294300	-0.151500
C	-2.726600	5.609200	-0.414500
H	-1.696300	5.535000	-0.760100
H	-2.732700	5.799100	0.657600
H	-3.256400	6.392900	-0.946200
C	-4.181900	-0.214400	-1.112500
C	-6.225500	-1.244500	-0.667800
H	-6.578200	-1.173700	-1.695500
H	-7.043800	-1.108300	0.032000
H	-5.742200	-2.208500	-0.511000
C	3.006200	0.705500	-1.618600
H	3.096900	-0.207900	-2.212000
C	4.495100	-0.126300	0.145600
C	4.870000	-1.415400	-0.261800
C	6.149900	-1.868100	0.047500
H	6.451400	-2.857900	-0.275100
C	7.028000	-1.093300	0.781400
H	8.017200	-1.462800	1.019400
C	6.621000	0.151300	1.238800
H	7.300700	0.734800	1.844300
C	5.363800	0.658500	0.933400
C	3.909600	-2.358200	-0.962700
H	2.949800	-1.855700	-1.068000
C	4.407000	-2.748400	-2.355400
H	4.590700	-1.869100	-2.975400
H	3.672700	-3.378800	-2.860000
H	5.342100	-3.308900	-2.291100
C	3.651300	-3.602500	-0.109500
H	4.565300	-4.182500	0.033400
H	2.915000	-4.245600	-0.595500
H	3.267700	-3.324000	0.873200

C 4.939200 2.028400 1.442600
H 3.912200 1.947500 1.814500
C 4.963200 3.076300 0.324000
H 4.657200 4.050500 0.709200
H 4.300400 2.819700 -0.501800
H 5.975900 3.167800 -0.074200
C 5.772000 2.527300 2.621000
H 6.788300 2.778800 2.311500
H 5.830000 1.785100 3.417900
H 5.322000 3.433400 3.028200
As 0.511300 -0.689500 0.092100
H 3.767700 1.400000 -1.993500
H 2.959800 1.166600 0.356300
92
11_As (isomer 2)
O -5.418200 -0.059200 -1.302700
N -1.784800 -0.546600 0.297400
C 0.454400 0.317200 -0.481000
O -3.762500 -1.228600 -2.255000
N 4.186500 0.260200 -0.844200
C -0.669800 0.851200 -1.162000
O -3.050400 4.271400 -1.676000
C -0.481400 1.751400 -2.239900
H -1.335300 2.128500 -2.790100
C 0.785000 2.114500 -2.591900
H 0.942700 2.796800 -3.417000
O -2.106600 3.320700 0.116800
C 1.908500 1.598900 -1.898300
H 2.904300 1.905700 -2.191300
C 1.762200 0.711600 -0.865400
C -1.901100 0.367700 -0.676800
C -3.660400 -0.332600 1.847400
C -2.939500 -1.120000 0.939100
C -4.799400 -0.885900 2.426000
H -5.372600 -0.299000 3.132700
C -5.203700 -2.172800 2.118500
H -6.094400 -2.585200 2.575300
C -4.460900 -2.939900 1.235900
H -4.776700 -3.951500 1.015200
C -3.312800 -2.438100 0.629100
C -3.204500 1.050300 2.265300
H -2.442400 1.401200 1.571800
C -4.340900 2.072400 2.242800
H -3.934600 3.072900 2.395400
H -5.069300 1.883300 3.033900
H -4.868200 2.057100 1.287000
C -2.567200 0.982200 3.656700
H -1.716200 0.299200 3.664000
H -3.293000 0.633700 4.395200
H -2.216500 1.970400 3.959200

C	-2.494100	-3.330400	-0.283400
H	-1.855500	-2.693500	-0.897100
C	-3.350900	-4.176100	-1.226200
H	-4.054400	-3.560200	-1.783400
H	-3.901700	-4.947000	-0.684000
H	-2.703700	-4.686100	-1.941500
C	-1.604200	-4.251200	0.560900
H	-0.977500	-4.867800	-0.086100
H	-2.223000	-4.914300	1.170200
H	-0.954000	-3.687600	1.229500
C	-3.228800	0.801600	-1.138000
C	-3.629100	2.068800	-1.254000
H	-4.597000	2.285900	-1.688900
C	-2.830100	3.253900	-0.839100
C	-2.322400	5.468400	-1.389200
H	-1.252700	5.264500	-1.398500
H	-2.606700	5.854500	-0.411600
H	-2.588500	6.171300	-2.172100
C	-4.148200	-0.281900	-1.624000
C	-6.340800	-1.071600	-1.716500
H	-6.329300	-1.173100	-2.800400
H	-7.314500	-0.741800	-1.369200
H	-6.070700	-2.021800	-1.256400
C	2.936500	0.157000	-0.102600
H	3.036000	0.699100	0.839600
C	5.370000	-0.068600	-0.135700
C	5.809100	0.792600	0.883000
C	6.939600	0.441000	1.615200
H	7.275800	1.091300	2.414700
C	7.659700	-0.702100	1.320700
H	8.540300	-0.958400	1.895500
C	7.263600	-1.501600	0.259300
H	7.856200	-2.371700	0.010800
C	6.123200	-1.210300	-0.480800
C	5.143300	2.129700	1.157400
H	4.334000	2.261300	0.439300
C	4.567600	2.207500	2.573000
H	3.858600	1.401700	2.769500
H	4.055600	3.159200	2.725400
H	5.364100	2.133400	3.316500
C	6.131100	3.276800	0.923700
H	6.962400	3.230400	1.629700
H	5.632200	4.238600	1.055800
H	6.542700	3.236400	-0.085500
C	5.698100	-2.108600	-1.632300
H	5.388000	-1.468500	-2.465300
C	4.509700	-2.993200	-1.238800
H	4.209700	-3.625300	-2.076500
H	3.643300	-2.410400	-0.928800
H	4.793000	-3.639700	-0.405600

C	6.824900	-2.984800	-2.174100
H	7.104600	-3.760100	-1.458500
H	7.713800	-2.399300	-2.411600
H	6.491300	-3.486600	-3.083200
As	-0.042700	-0.887200	0.864800
H	2.714800	-0.884400	0.179600
H	4.107600	-0.268200	-1.701500