Supporting Information

for

Isolation of Singlet Carbene Derived 2-Arsa-1,3-butadiene Radical Cations and Dications

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Materials and Methods

All the experiments and manipulations were carried out under an inert gas (Ar or N_2) atmosphere using standard *Schlenk* techniques or an MBraun LABmaster Pro glovebox. THF (Na/K), *n*-hexane (Na/K), and diethyl ether ($LiAlH_4$) were dried by refluxing over appropriate drying agents, distilled prior to use, and stored over molecular sieve (3Å). Starting materials, {(IPr)C(Ph)}$AsCl_2$ (**1**)[1] and cyclic alkyl amino carbenes (cAACs)[2] were synthesized according to literature methods. $GaCl_3$ was purchased from ABCR and used without further purification. NMR spectra were recorded using a Bruker Avance III 500HD NMR spectrometer. Chemical shifts are given in δ ppm and are referenced to the solvent residual peaks.[3] Melting points were measured using a Büchi B-545 melting point apparatus. UV-visible spectra were recorded using a Thermo Fisher Evolution 300 spectrophotometer. Infrared spectra were recorded using a Bruker Alpha-T FTIR spectrometer.

Synthesis of (L)As(cAAC^{Me}) 2a

To a *Schlenk* flask containing **1** (1.00 g, 1.60 mmol), cAAC^{Me} (0.71 g, 1.60 mmol), and Mg turnings (0.11 mg, 4.80 mmol) was added 20 mL THF at room temperature (rt). The resulting reaction mixture was stirred overnight at rt. During this period, the initially green solution resulted in an orange solution. The volatiles were removed in vacuo. The orange residue was extracted with 50 mL *n*-hexane, filtered through a plug of Celite, and the filtrate was dried under vacuum to obtain **2a** as an orange solid. Yield: 1.21 g, 90%. Mp: 132 °C (dec.). X-ray quality single crystals were grown by cooling a saturated *n*-pentane solution of **2a** at –40 °C. Elemental analysis (%), calcd for **2a**, $C_{54}H_{72}AsN_3$ (838.09): C, 77.39; H, 8.66; N, 5.01; found: C, 77.97; H, 8.97; N, 5.23. ^{1}H NMR (500 MHz, C_6D_6, 298 K): δ = 7.10–7.16 (m, 9H, C_6H_3), 6.86 (br, 2H, C_6H_5), 6.73 (t, J = 7.5 Hz, 2H, C_6H_5), 6.62 (t, 1H, J = 7.2 Hz, C_6H_5), 5.81 (br, 1H, NC*H*), 5.70 (br, 1H, NC*H*), 3.73 (br, 2H, C*H*$(CH_3)_2$), 3.41 (br, 2H, C*H*$(CH_3)_2$), 2.82 (m, 2H, C*H*$(CH_3)_2$), 1.71 (s, 1H, CH_2), 1.38 (br, 12H, CH(C*H*$_3)_2$), 1.32 (br, 6H, CH(C*H*$_3)_2$), 1.23 (br, 6H, CH(C*H*$_3)_2$), 1.17 (d, J = 6.7 Hz, 6H, CH(C*H*$_3)_2$), 1.11 (d, J = 6.3 Hz, 6H, C*H*$_3$), 0.95 (s, 6H, C*H*$_3$) ppm. ^{13}C{^{1}H} NMR (125 MHz, C_6D_6, 298 K): δ = 220.0 (C_{cAAC}); 148.5, 147.2, 147.0, 146.6, 146.2, 138.7, 135.4, 133.6 (C_6H_3); 126.2, 125.0, 124.8, 123.6, 122.3, 119.2, 118.2 (C_6H_5); 78.0 (*C*Ph); 68.0, 56.9 (N*C*$(CH_3)_2$, *C*$(CH_3)_2$); 51.2 (CH_2); 29.5, 29.3, 29.1, 28.7 (*C*H$(CH_3)_2$; 26.1, 25.6, 24.5, 23.4, 22.6 (*C*H$_3$). UV/vis (THF, λ (nm) (ε (M^{-1} cm^{-1})): 222 (23300), 268 (10300), 368 (10100), 438 (7750).

Synthesis of (L)As(cAAC^{Cy}) 2b

Compound **2b** was synthesized following a similar protocol as described for compound **2a**, using compound **1** (1.00 g, 1.60 mmol), cAAC^{Cy} (0.77 g, 1.60 mmol), and Mg turnings (0.11 mg, 4.80 mmol). Yield: 1.3 g, 93%; orange solid. Mp: 129 °C (dec.). Elemental analysis (%), calcd for **2b**, $C_{57}H_{76}AsN_3$ (878.16): C, 77.96; H, 8.72; N, 4.79; found: C, 78.27; H, 8.97; N, 4.89. ^{1}H NMR

(500 MHz, C_6D_6, 298 K): δ = 7.27 (d, J = 7.1 Hz, 2H, C_6H_3), 7.16–7.20 (m, 2H, C_6H_3), 7.12 (d, J = 7.4 Hz, 3H, C_6H_3), 7.07 (br, 2H, C_6H_3), 6.85 (br, 2H, C_6H_5), 6.78 (t, J = 7.2 Hz, 2H, C_6H_5), 6.58 (t, J = 7.0 Hz,1H, C_6H_5), 5.79 (br, 1H, NC*H*), 5.67 (br, 1H, NC*H*), 3.71 (br, 2H, C*H*$(CH_3)_2$), 3.47 (br, 2H, C*H*$(CH_3)_2$), 2.84 (m, 2H, C*H*$(CH_3)_2$), 1.74 (s, 1H, CH_2), 1.53 (br, 4H, Cy), 1.36 (br, 12H, CH(C*H*$_3)_2$), 1.22 (br, 12H, CH(C*H*$_3)_2$), 1.19 (d, J = 6.6 Hz, 12H, CH(C*H*$_3)_2$), 1.12 (br, 6H, C*H*$_3$), 0.95 (s, 6H, C*H*$_3$) ppm. $^{13}C\{^1H\}$ NMR (125 MHz, C_6D_6, 298 K): δ = 219.8 (C_{cAAC}); 149.3, 148.5, 147.3, 146.3, 145.1, 135.3, 133.7 (C_6H_3); 127.1, 125.1, 124.5, 123.6, 122.5, 119.1, 118.7 (C_6H_5); 79.7 (*C*Ph); 68.0, 56.4 (N*C*$(CH_3)_2$, *C*$(CH_3)_2$); 49.2 (CH_2); 34.3, 29.6, 29.2, 28.8 (CH(*C*$H_3)_2$; 26.0, 25.5, 24.8, 24.3, 23.6, 22.8, 14.3 (*C*H_3). UV/vis (THF, λ (nm) (ε (M^{-1} cm^{-1})): 238 (23040), 263 (16450), 321 (14960), 426 (16720).

Synthesis of [(L)As(cAAC^{Me})](GaCl$_4$) 3a

To a 20 mL diethyl ether solution of **2a** (200 mg, 0.24 mmol) was added $GaCl_3$ (84 mg, 0.48 mmol) at rt with constant stirring. After stirring overnight, the green precipitate was collected by filtration and dried in *vacuo* to afford **3a** as a dark green crystalline solid. Yield: 225 mg, 90%. Mp: 143 °C (dec.). Single crystals suitable for X-ray diffraction studies were grown by a slow diffusion of *n*-hexane into a saturated THF solution of **3a**. Elem. Anal. calcd. for **3a**, $C_{54}H_{72}AsCl_4GaN_3$ (1049.63): C, 61.79; H, 6.91; N, 4.00, found: C, C, 62.05; H, 7.22; N, 4.09. UV/vis (THF, λ (nm) (ε (M^{-1} cm^{-1})): 223 (23180), 337 (5970), 448 (3790), 616 (11440), 749 (6380).

Synthesis of [(L)As(cAAC^{Cy})](GaCl$_4$) 3b

Compound **3b** was synthesized by following a similar protocol as described for compound **3a**, using compound **2b** (400 mg, 0.45 mmol), and $GaCl_3$ (160 mg, 0.90 mmol) as a dark green solid. Yield: 410 mg, 83%. Mp: 142 °C (dec.). Single crystals suitable for X-ray diffraction studies were grown by a slow diffusion of *n*-hexane into a saturated THF solution of **3b**. Elem. Anal. calcd. for **3b**, $C_{57}H_{76}AsCl_4GaN_3$ (1089.69): C, 62.83; H, 7.03; N, 3.86, found: C, 63.19; H, 7.45; N, 3.97. UV/vis (THF, λ (nm) (ε (M^{-1} cm^{-1})): 235 (25770), 338 (9820), 452 (6810), 629 (18880), 757 (11010).

Synthesis of [(L)As(cAAC^{Me})](GaCl$_4$)$_2$ 4a

To a DCM solution (10 mL) of **3a** (50 mg, 0.05 mmol) was transferred $GaCl_3$ (17 mg, 0.10 mmol) at rt. The color of the solution turned green to yellow immediately, which was further stirred for 2h. The volatiles were removed in *vacuo* to afford **6** as a yellow solid. Yield: 60 mg, 99%. Mp: 139 °C (dec.). Single crystals of **4a** suitable for X-ray diffraction were grown by a slow diffusion of *n*-hexane into a saturated dichloromethane solution of **4a**. Elem. Anal. calcd. for **4a**, $C_{54}H_{72}AsCl_8Ga_2N_3$ (1261.16): C, 51.43; H, 5.75; N, 3.33; found: C, 51.73; H, 5.97; N, 3.49. ^1H NMR (500 MHz, CD_2Cl_2, 298 K): δ = 7.95 (s, 2H, NC*H*), 7.68–7.72 (m, 2H, C_6H_3), 7.60 (t, J = 7.8 Hz, 2H, C_6H_3), 7.43–7.50 (m, 5H, C_6H_3, C_6H_5), 7.28 (d, J = 7.8 Hz, 4H, C_6H_3, C_6H_5), 6.71 (d, J = 7.7 Hz, 2H, C_6H_5), 2.55 (m, 2H, C*H*$(CH_3)_2$), 2.35 (s, 2H, CH_2), 2.28 (m, 4H, C*H*$(CH_3)_2$), 1.57 (s, 6H, C*H*$_3$), 1.33 (d, J = 6.5 Hz, 6H,

CH(CH_3)$_2$), 1.18 (d, J = 6.7 Hz, 12H, CH(CH_3)$_2$), 1.14 (d, 6H, J = 6.6 Hz, CH(CH_3)$_2$), 0.98 (d, J = 6.7 Hz, 12H, CH(CH_3)$_2$), 0.63 (s, 6H, CH_3) ppm. ^{13}C{^{1}H} NMR (125 MHz, CD_2Cl_2, 298 K): δ = 221.1 (C_{cAAC}); 187.5, 147.4, 146.2, 145.2, 143.5, 135.3, 134.2, 131.8, 131.4 (C_6H_3); 129.0, 128.8, 128.0, 126.0 (C_6H_5); 87.2 (C(CH$_3$)$_2$; 74.2 (C(CH$_3$)$_2$; 58.2, 52.8 (CH_2); 30.5, 27.4, 26.7, 25.8, 25.4 (CH(CH$_3$)$_2$; 22.3 (CH_3) ppm. UV/vis (THF, λ (nm) (ε (M^{-1} cm^{-1})): 241 (24940), 265 (20500), 330 (17300), 389 (18090).

One-pot Synthesis of 4a

To a DCM solution (5 mL) of **2a** (0.15 g, 0.18 mmol), was transferred $GaCl_3$ (126 mg, 0.72 mmol) at rt. The color of the solution turned yellow immediately, which was further stirred for 2 h. Removal of volatiles afforded **4a** as a yellow solid. Yield: 223 mg, 99%.

Synthesis of [(L)As(cAAC^{Cy})](GaCl$_4$)$_2$ 4b

Compound **4b** was synthesized following the similar protocol as described for compound **4a**, using compound **3b** (110 mg, 0.10 mmol), and $GaCl_3$ (36 mg, 0.20 mmol). Yield: 128 mg, 98%, yellow solid. Mp: 143 °C (dec.). Single crystals of **4b** suitable for X-ray diffraction were grown by a slow diffusion of *n*-hexane into a saturated dichloromethane solution of **7**. Elem. Anal. calcd. for **4b**, $C_{57}H_{76}AsCl_8Ga_2N_3$ (1301.23): C, 52.61; H, 5.89; N, 3.23; found: C, 52.93; H, 6.27; N, 3.37. ^{1}H NMR (500 MHz, CD_2Cl_2, 298 K): δ = 7.99 (s, 2H, NCH), 7.73–7.68 (m, 2H, C_6H_3), 7.61 (t, J = 7.8 Hz, 2H, C_6H_5), 7.48 (t, J = 9.1 Hz, 4H, C_6H_3), 7.30 (d, J = 7.8 Hz, 4H, C_6H_5), 6.79 (d, J = 7.7 Hz, 2H, C_6H_5), 2.59 (br, 2H, CH(CH$_3$)$_2$), 2.34 (br, 6H, CH_2, CH(CH$_3$)$_2$), 1.58 (s, 6H, CH_3), 1.38-1.44 (m, 3H, CH_2), 1.33 (d, J = 6.4 Hz, 6H, CH(CH_3)$_2$), 1.18 (d, J = 6.4 Hz, 12H, CH(CH_3)$_2$), 1.12-1.14 (m, 3H, CH_2), 0.97 (br, 6H, CH(CH_3)$_2$), 0.92 (d, J = 6.4 Hz, 12H, CH(CH_3)$_2$), 0.33 (br, 3H, CH_3) ppm. ^{13}C{^{1}H} NMR (125 MHz, CD_2Cl_2, 298 K): δ = 220.2 (C_{cAAC}); 186.6, 147.0, 146.4, 145.4, 142.9, 135.5, 134.0, 131.3, 131.1 (C_6H_3); 129.1, 128.7, 128.4, 126.1 (C_6H_5); 87.1 (C(CH$_3$)$_2$; 74.2 (C(CH$_3$)$_2$; 63.8, 46.2 (CH_2); 30.6, 30.4, 27.5 (CH(CH$_3$)$_2$; 26.2, 26.1, 25.8, 23.6, 22.5, 21.7 (CH_3) ppm. UV/vis (THF, λ (nm) (ε (M^{-1} cm^{-1})): 222 (20700), 265 (12740), 326 (6670), 402 (9501).

One-pot Synthesis of 4b

To a DCM solution (5 mL) of **2b** (0.15 g, 0.17 mmol), was transferred $GaCl_3$ (120 mg, 0.68 mmol) at rt. The color of the solution turned yellow immediately, which was further stirred for 2 h. Removal of volatiles afforded **4b** as a yellow solid. Yield: 217 mg, 98%.

Plots of the NMR spectra

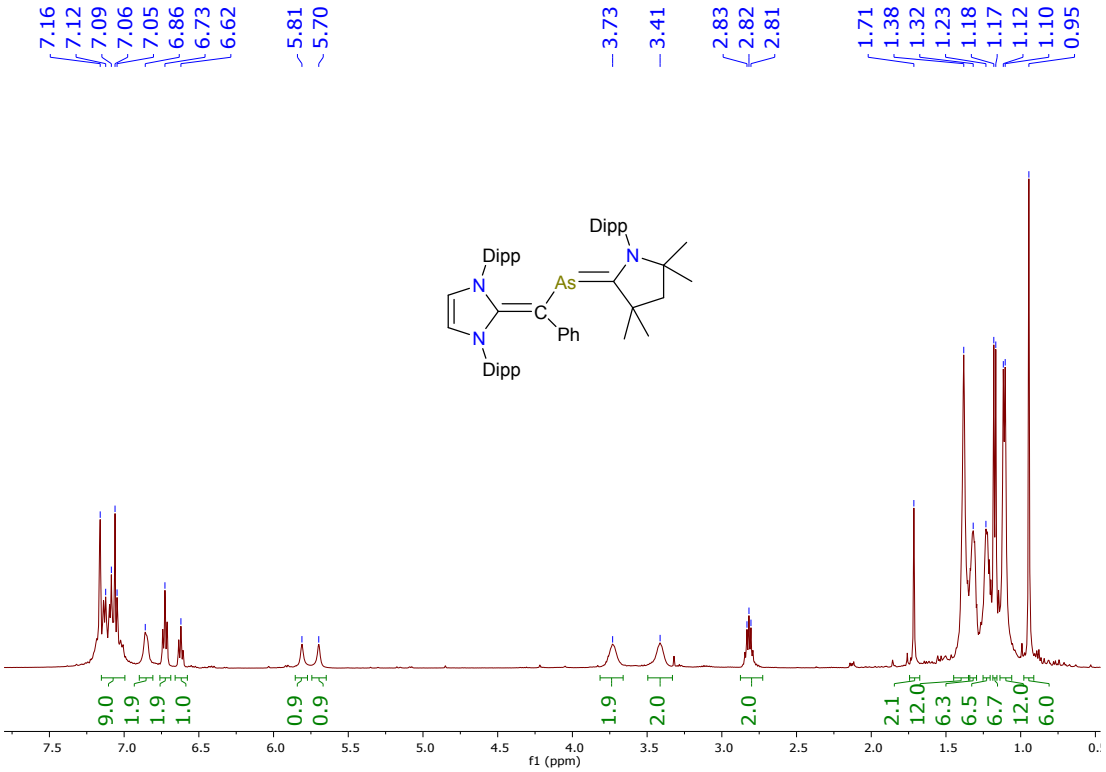


Figure S1. ^{1}H NMR spectrum (C_6D_6, 298 K, 500 MHz) of compound **2a**.

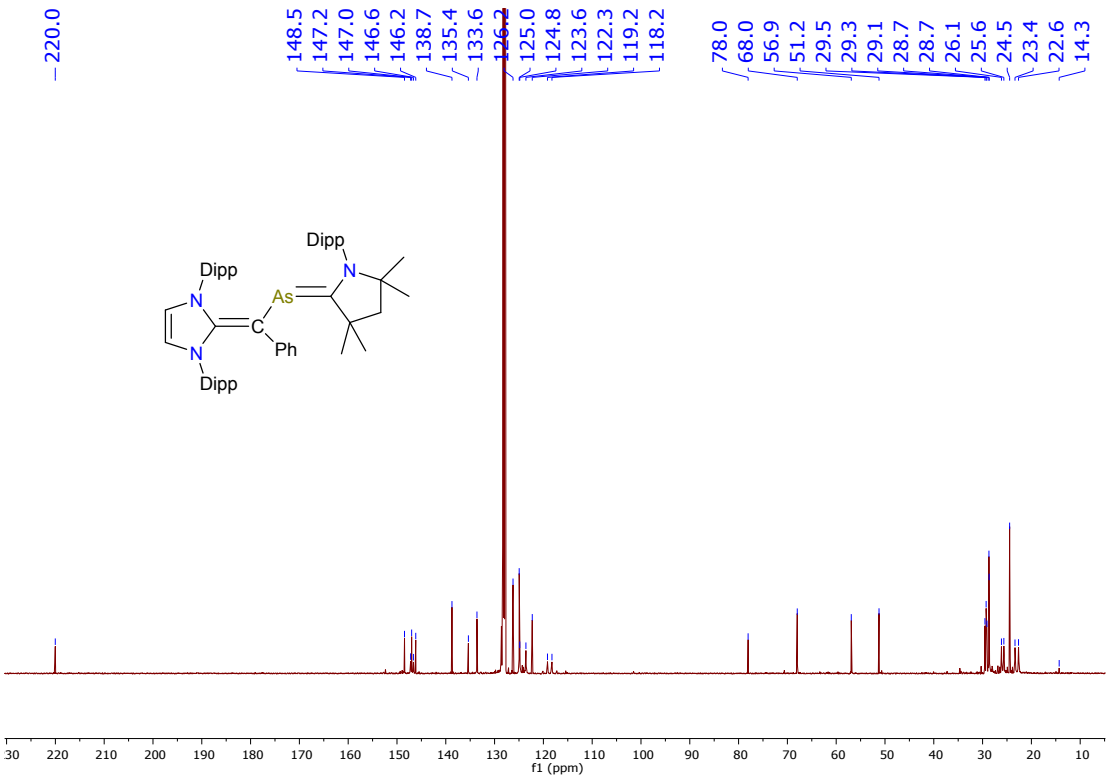


Figure S2. ^{13}C{^{1}H} NMR spectrum (C_6D_6, 298 K, 125 MHz) of compound **2a**.

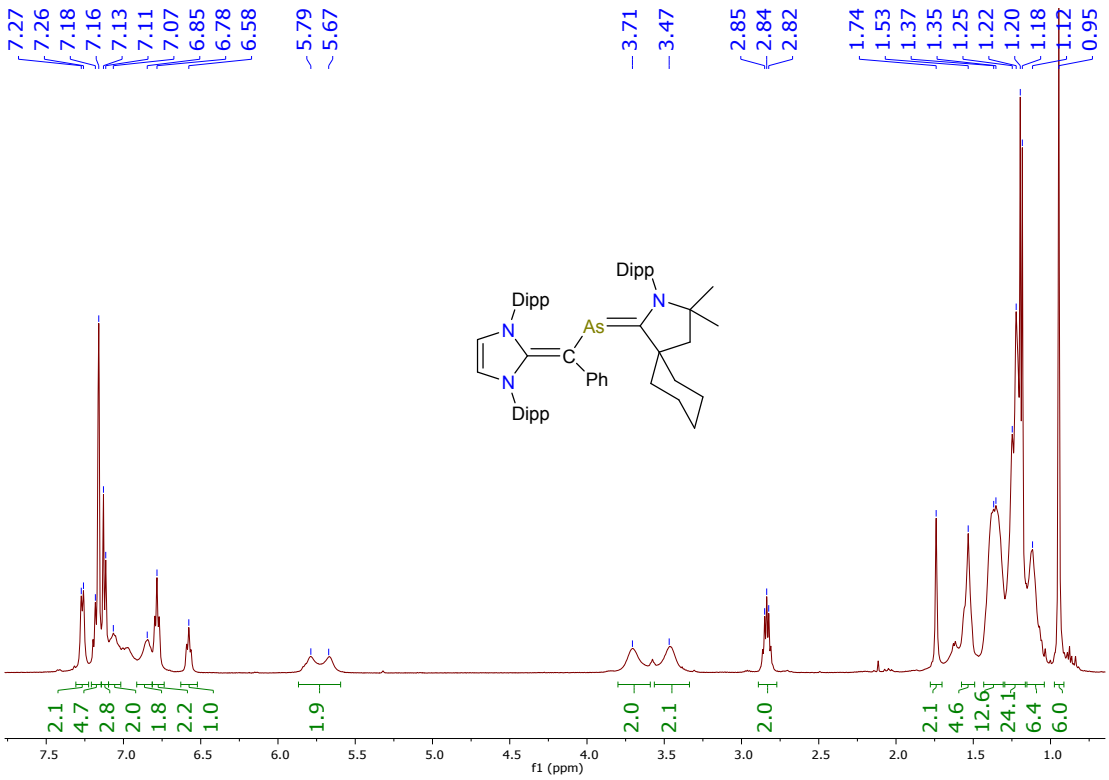


Figure S3. ^{1}H NMR spectrum (C_6D_6, 298 K, 500 MHz) of compound **2b**.

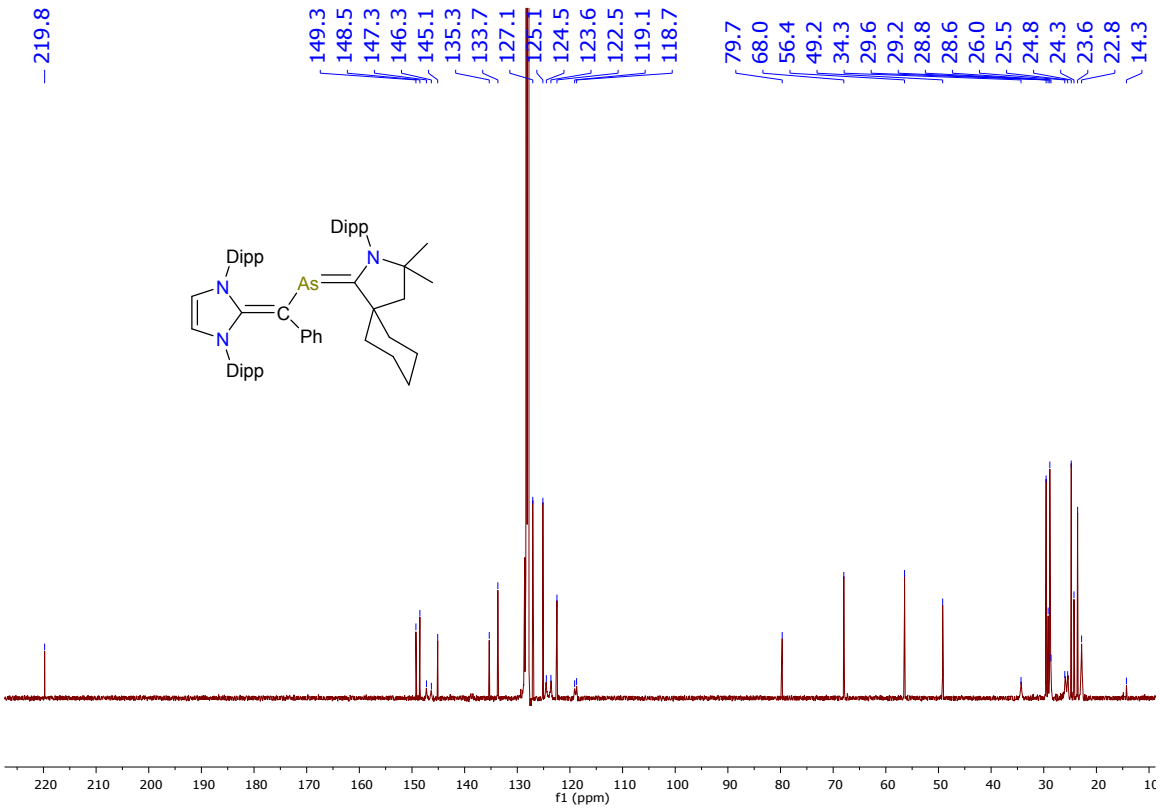


Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum (C_6D_6, 298 K, 125 MHz) of compound **2b**.

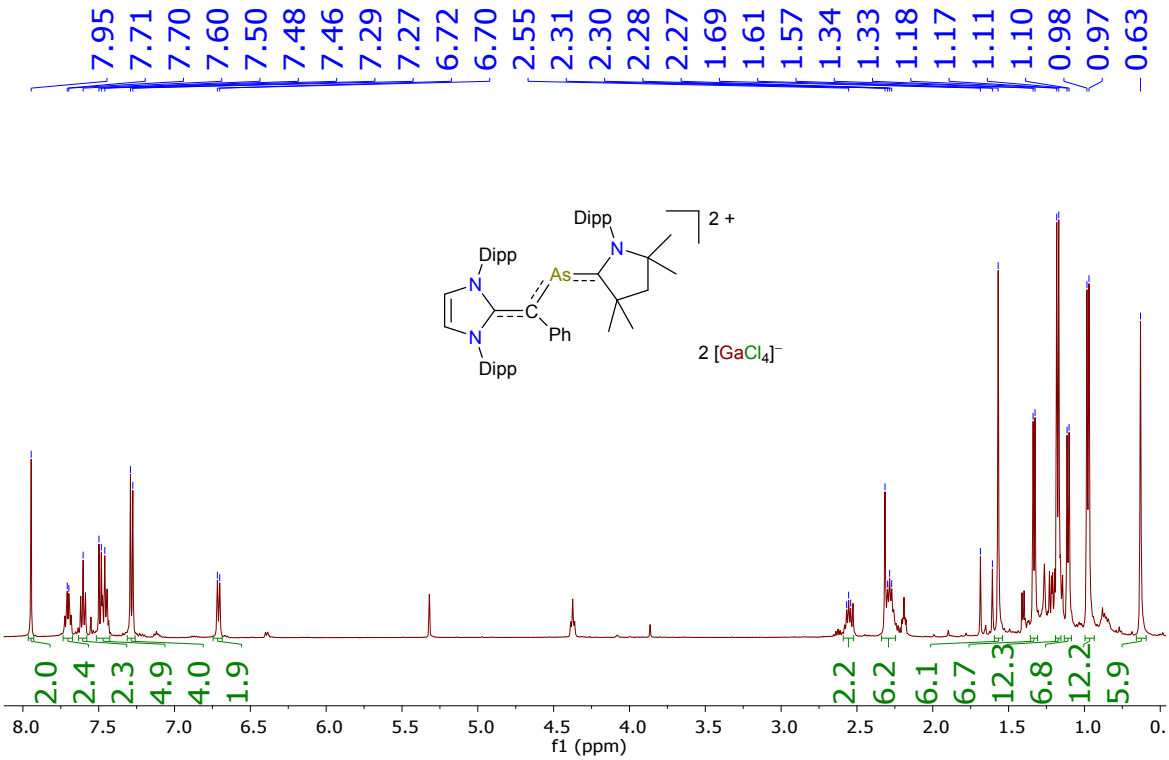


Figure S5. ^{1}H NMR spectrum (CD_2Cl_2, 298 K, 500 MHz) of compound **4a**.

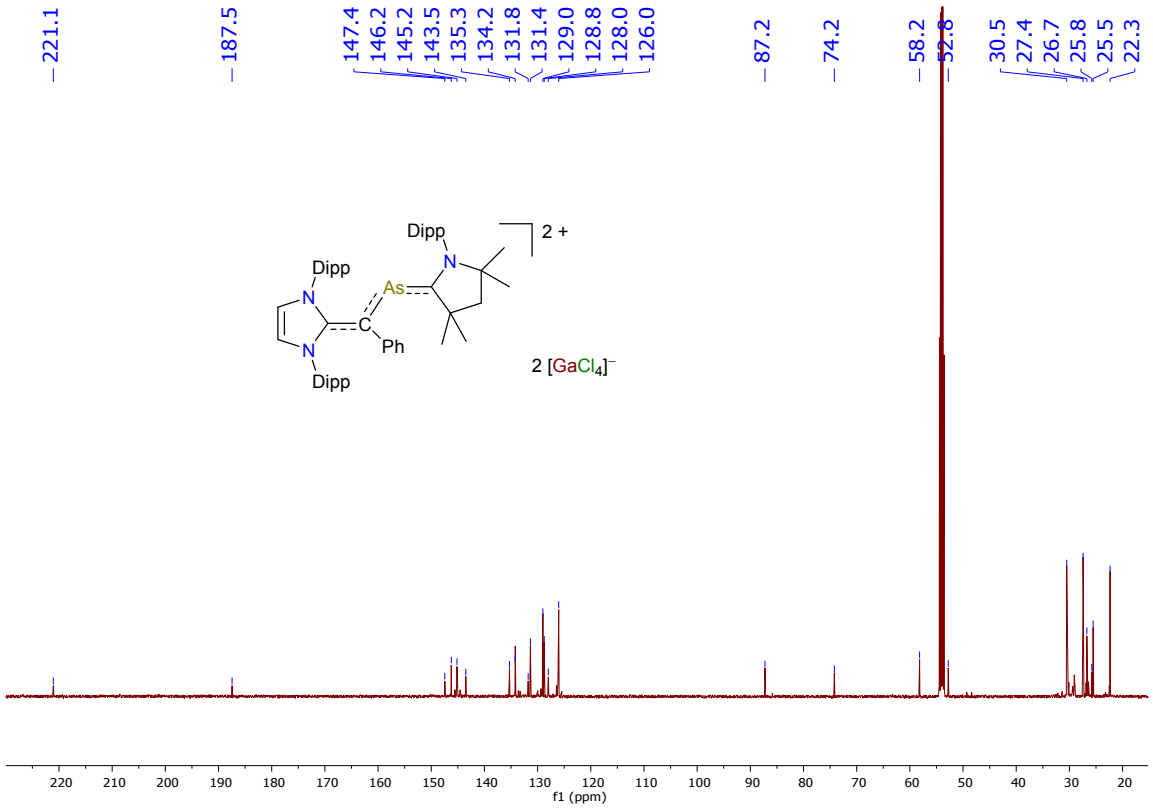


Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum (CD_2Cl_2, 298 K, 125 MHz) of compound **4a**.

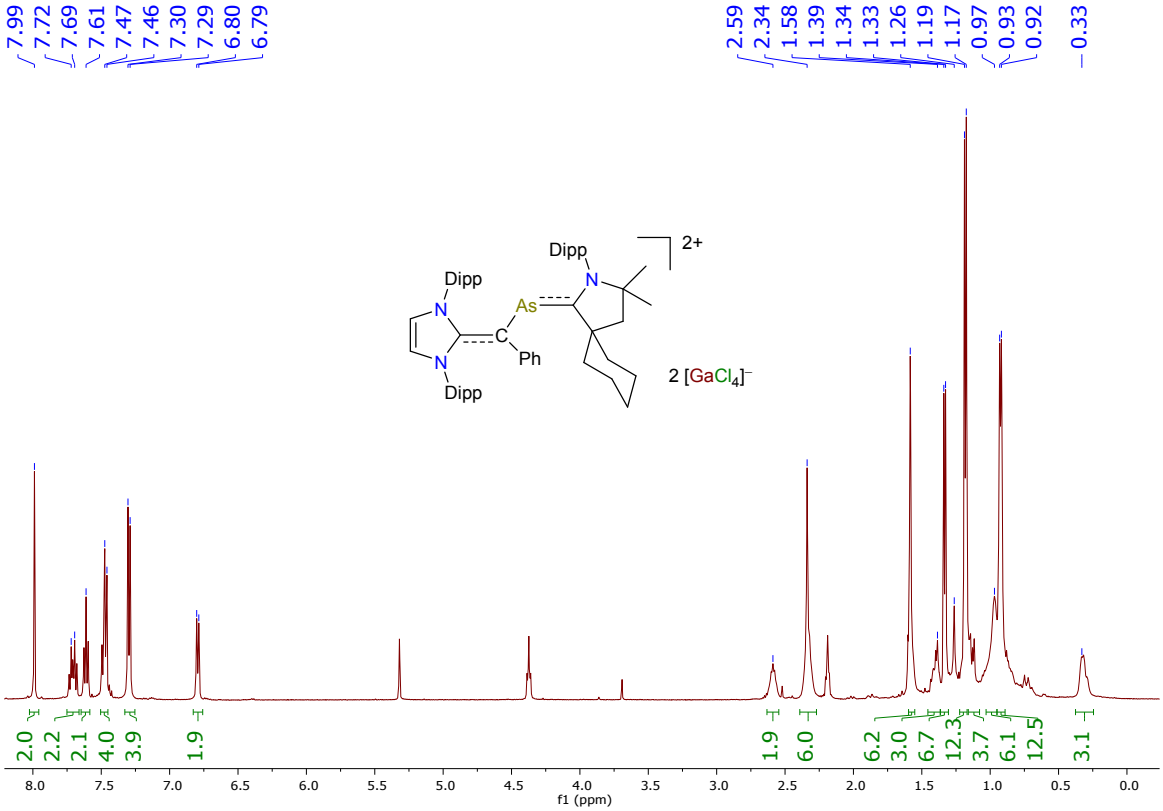


Figure S7. ^{1}H NMR spectrum (CD_2Cl_2, 298 K, 500 MHz) of compound **4b**.

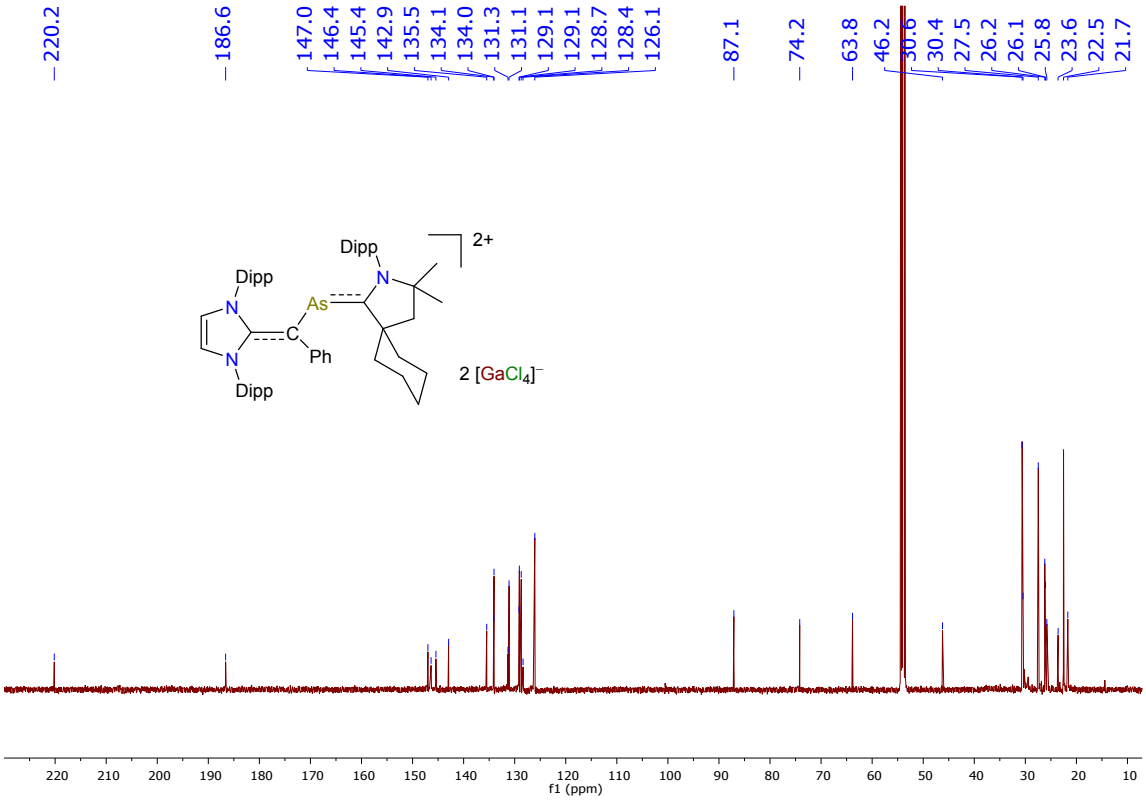


Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum (CD_2Cl_2, 298 K, 125 MHz) of compound **4b**.

Plots of the IR spectra

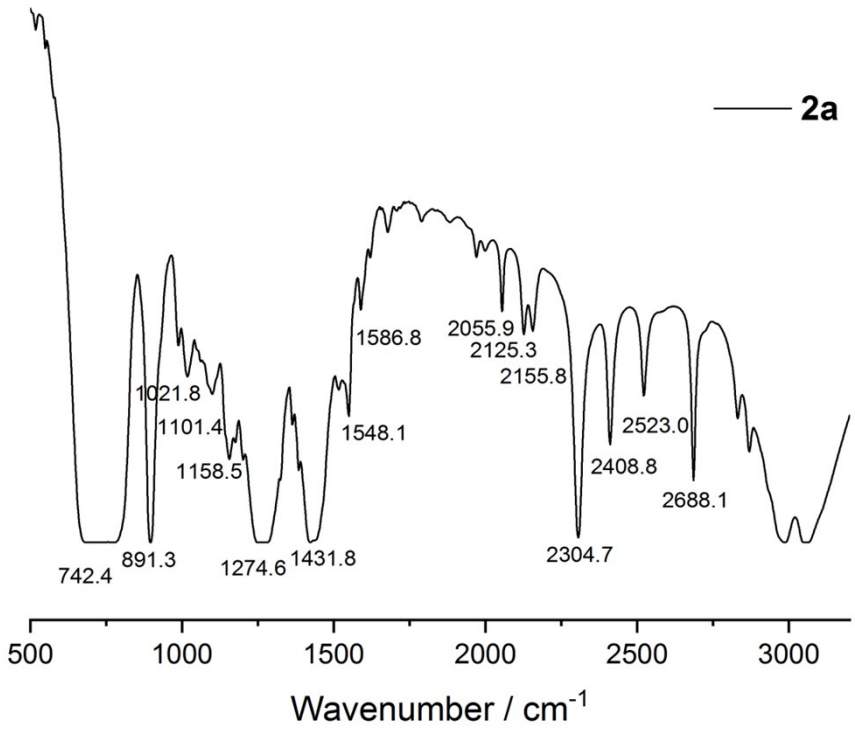


Figure S9. Solution IR spectrum (CH_2Cl_2, 298 K) of compound **2a**.

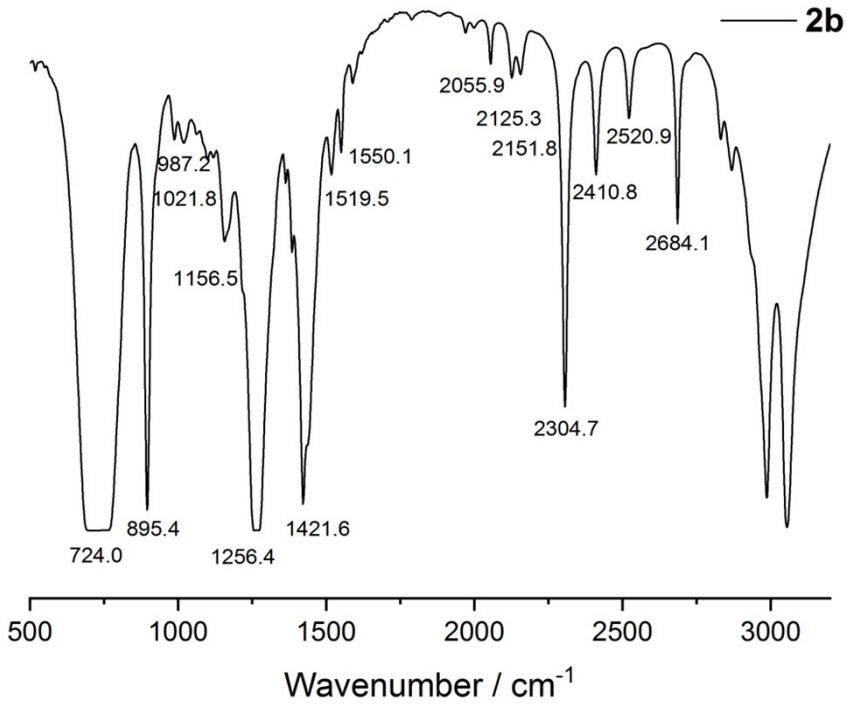


Figure S10. Solution IR spectrum (CH_2Cl_2, 298 K) of compound **2b**.

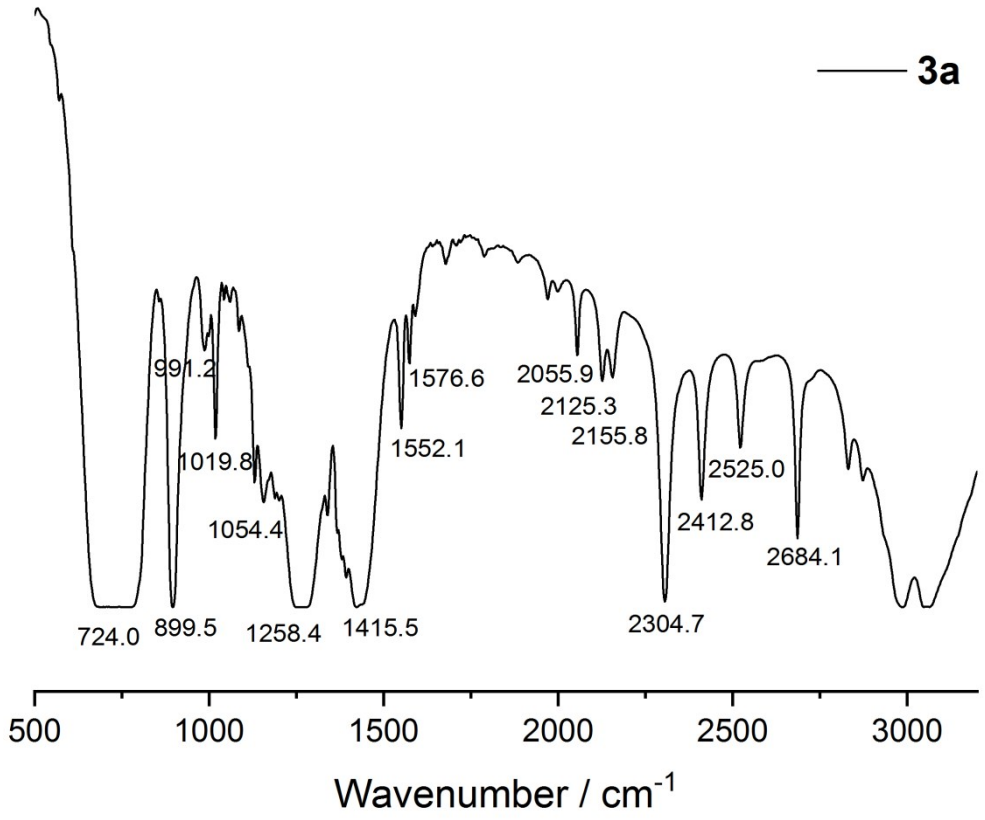


Figure S11. Solution IR spectrum (CH_2Cl_2, 298 K) of compound **3a**.

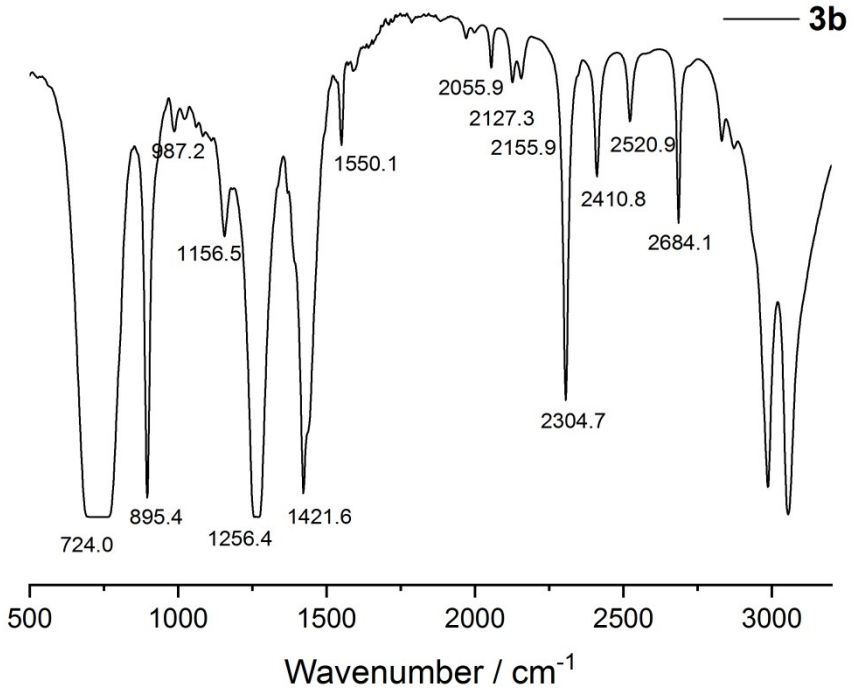


Figure S12. Solution IR spectrum (CH_2Cl_2, 298 K) of compound **3b**.

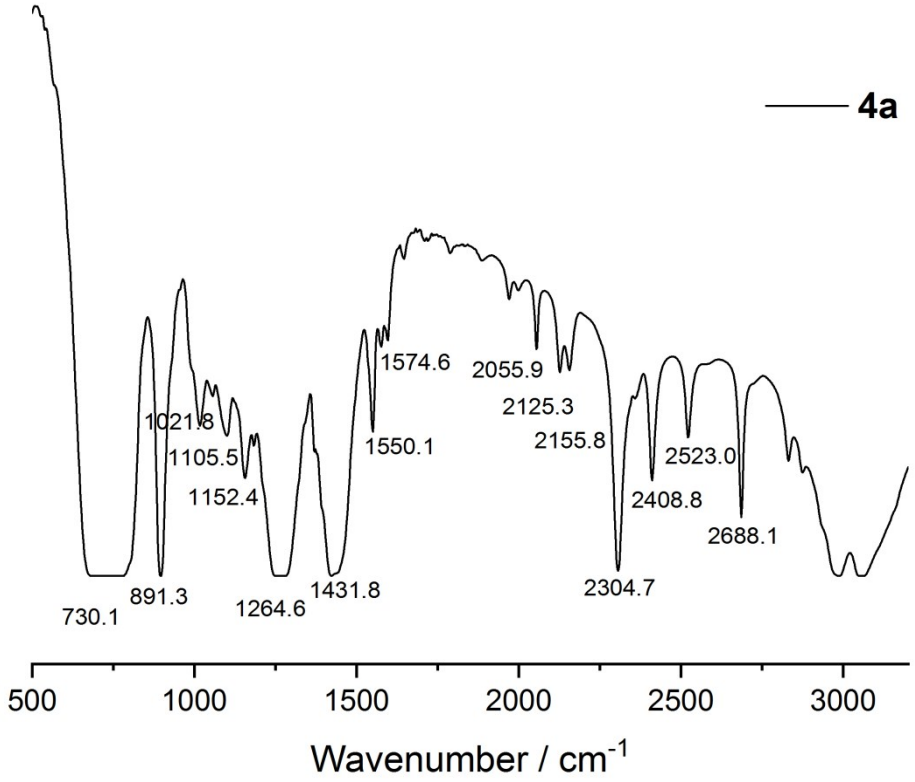


Figure S13. Solution IR spectrum (CH_2Cl_2, 298 K) of compound **4a**.

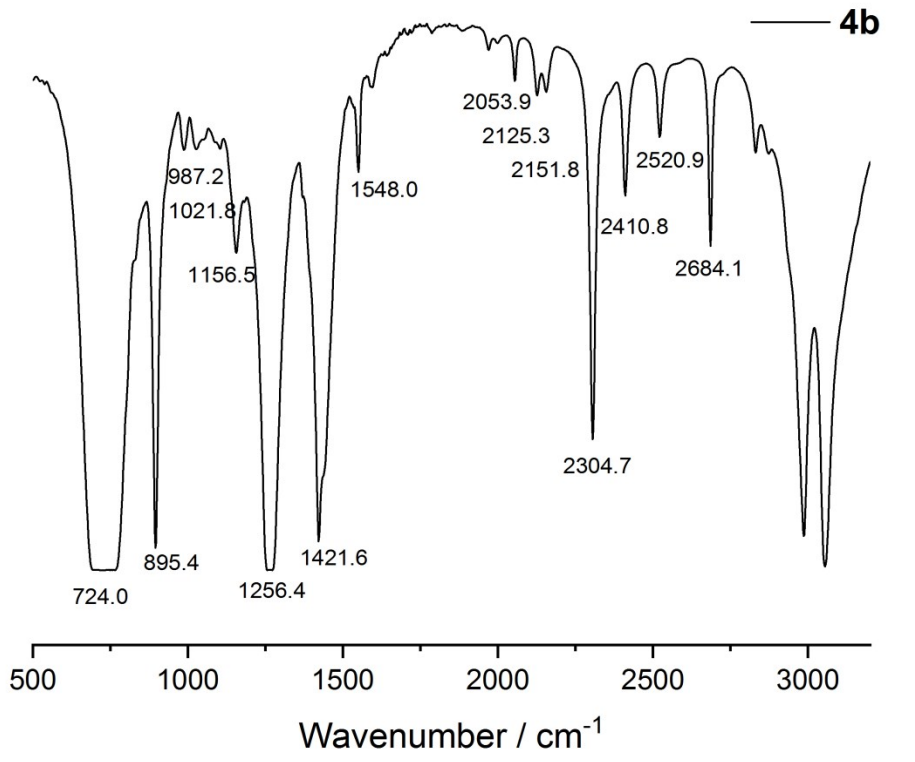


Figure S14. Solution IR spectrum (CH_2Cl_2, 298 K) of compound **4b**.

Cyclic Voltammetry

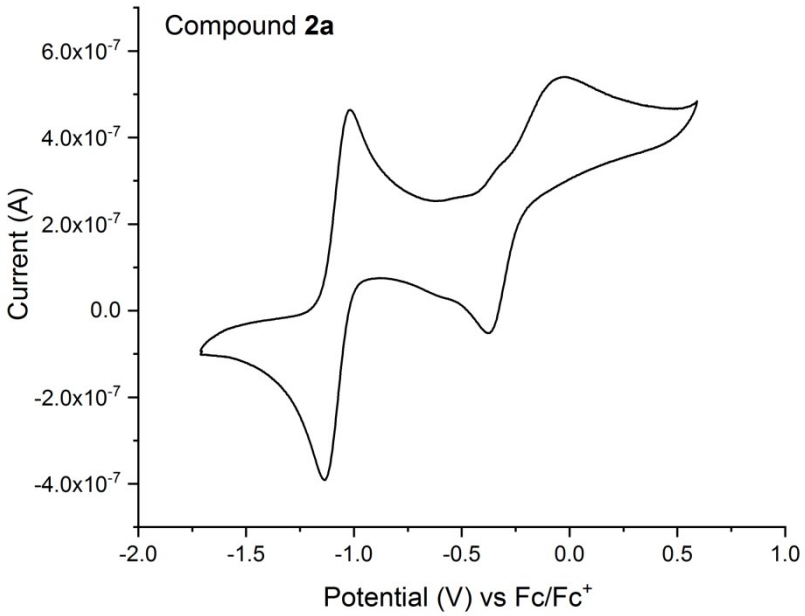


Figure S15. Cyclic voltammogram of **2a** in DCM (0.01 M *n*-$Bu_4N[Al(OC(CF_3)_3]_4$ as a supporting electrolyte, 100mVs^{-1}, *vs* Fc/Fc^+). The cycle for Fc/Fc^+ couple has been removed for clarity.

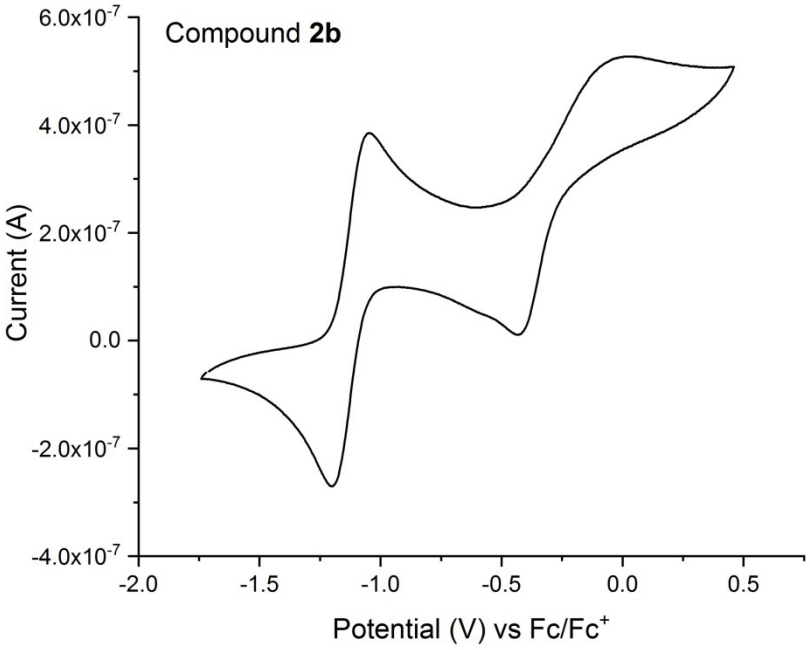


Figure S16. Cyclic voltammogram of **2b** in DCM (0.01 M *n*-$Bu_4N[Al(OC(CF_3)_3]_4$ as a supporting electrolyte, 100mVs^{-1}, *vs* Fc/Fc^+). The cycle for Fc/Fc^+ couple has been removed for clarity.

UV-vis Spectroscopy

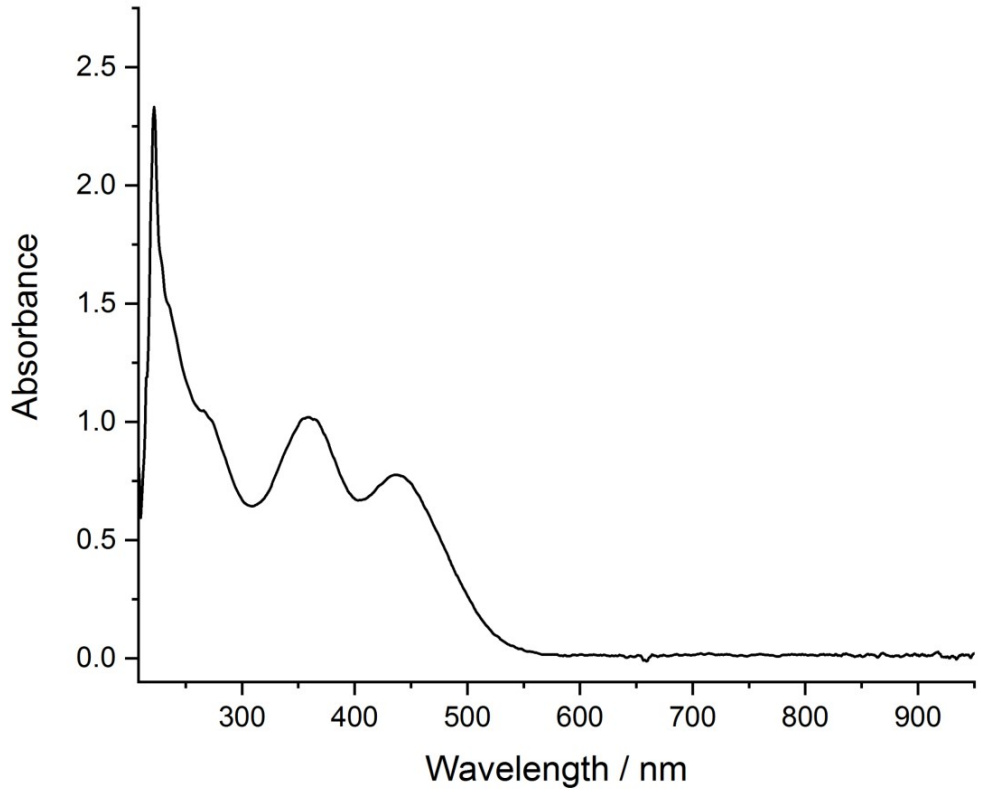


Figure S17. UV-visible spectrum of **2a** (10^{-4} M) recorded in THF.

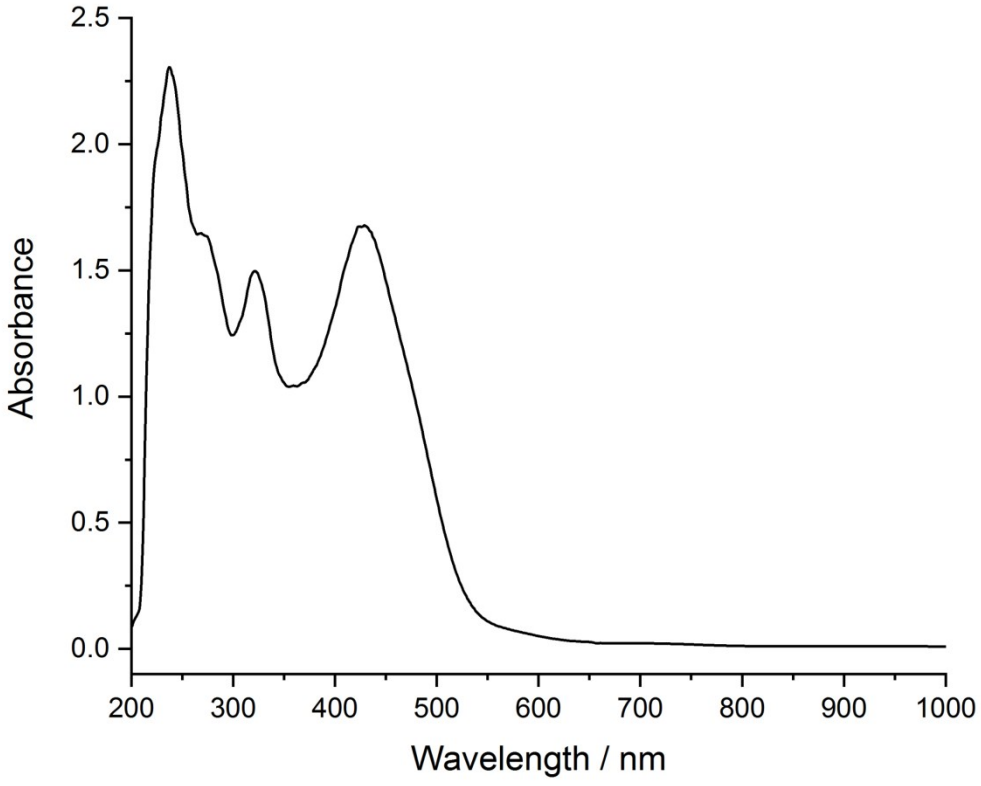


Figure S18. UV-visible spectrum of **2b** (10^{-4} M) recorded in THF.

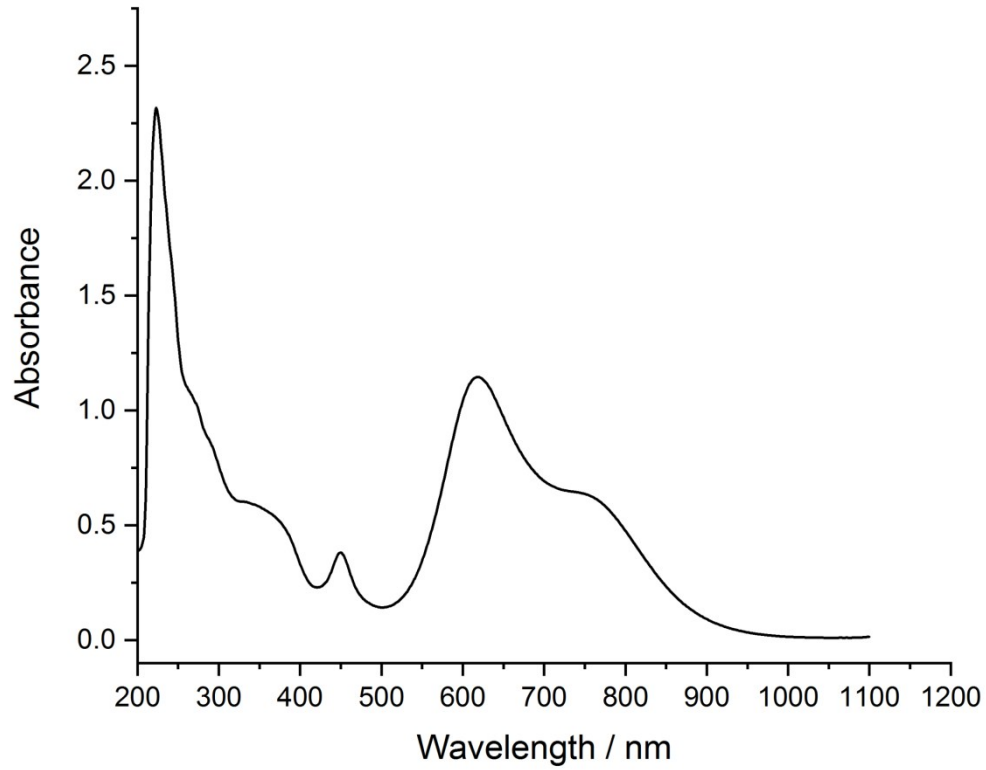


Figure S19. UV-visible spectrum of **3a** (10^{-4} M) recorded in THF.

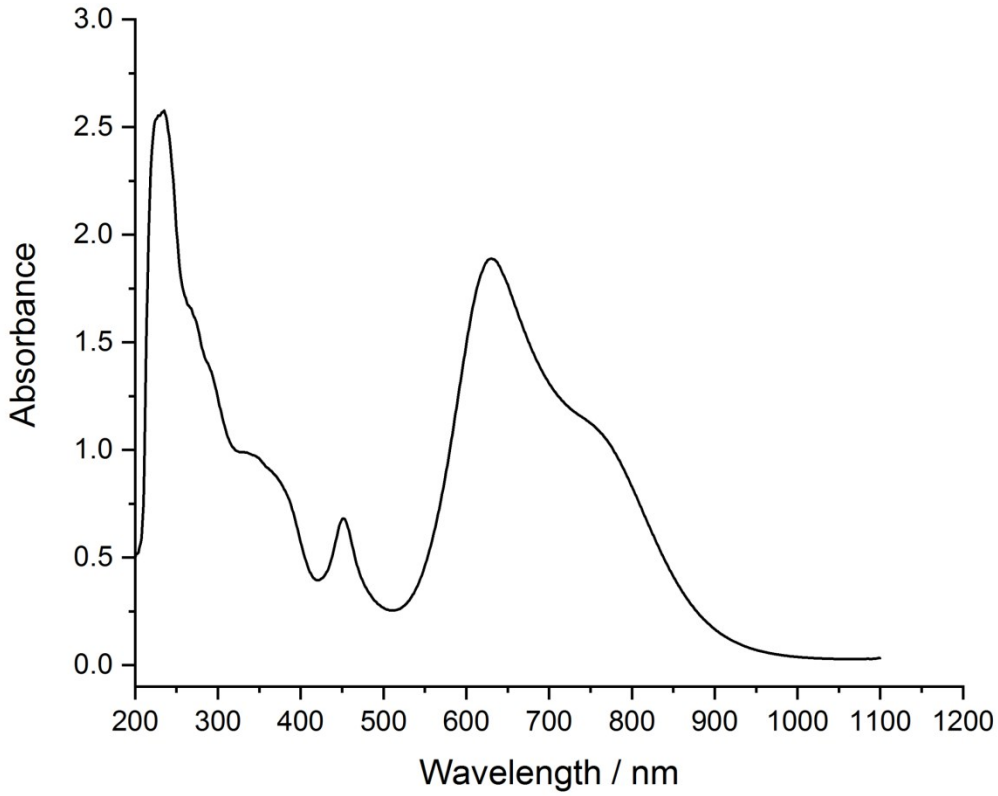


Figure S20. UV-visible spectrum of **3b** (10^{-4} M) recorded in THF.

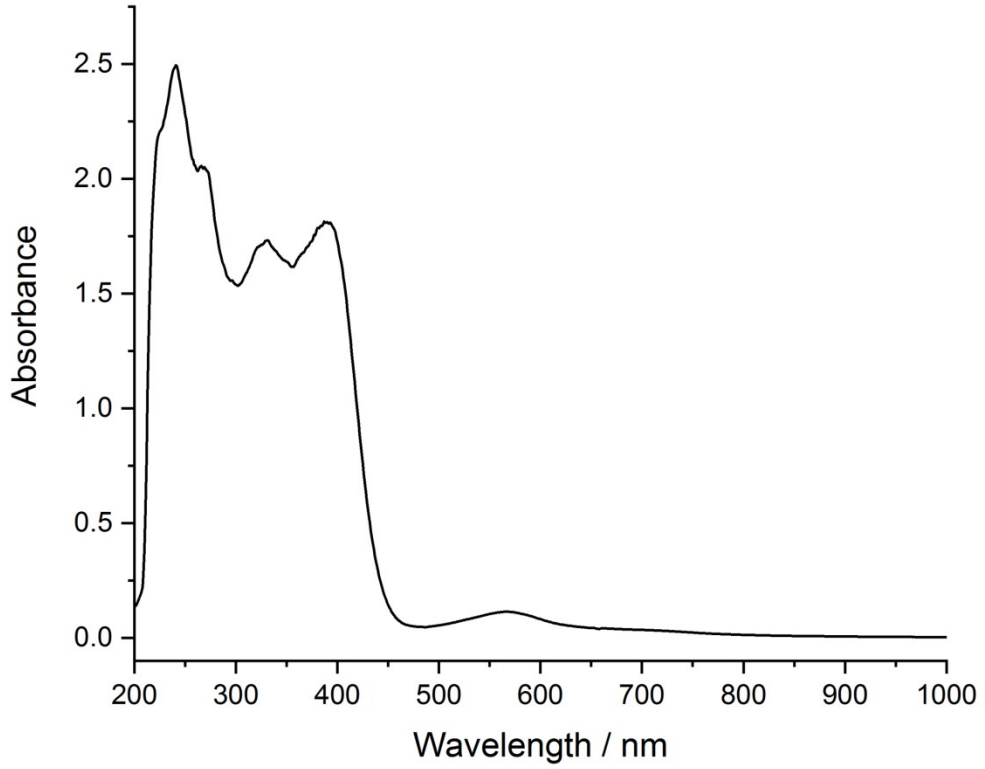


Figure S21. UV-visible spectrum of **4a** (10^{-4} M) recorded in THF.

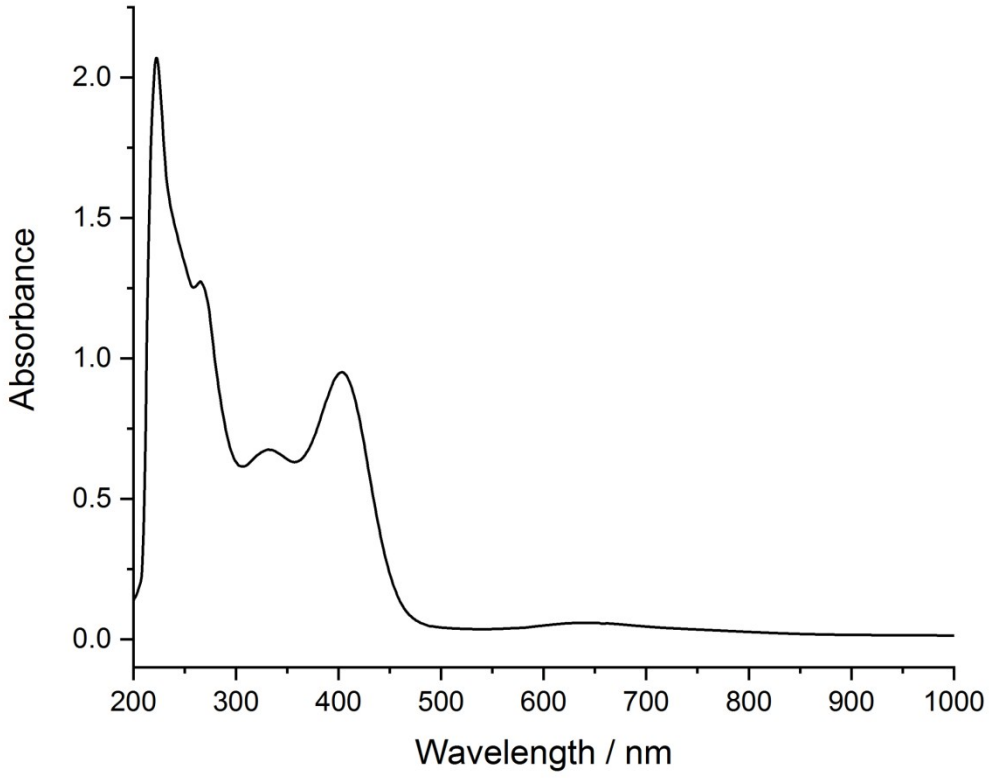


Figure S22. UV-visible spectrum of **4b** (10^{-4} M) recorded in THF.

EPR Spectroscopy

The continuous wave (CW) EPR experiments were performed at room temperature (298 K) as well as at 80 K on a Bruker standard ST9402 resonator and with a Bruker ELEXSY E500 spectrometer. The microwave frequency was 9.628 GHz and the modulation amplitude was 0.3 mT.

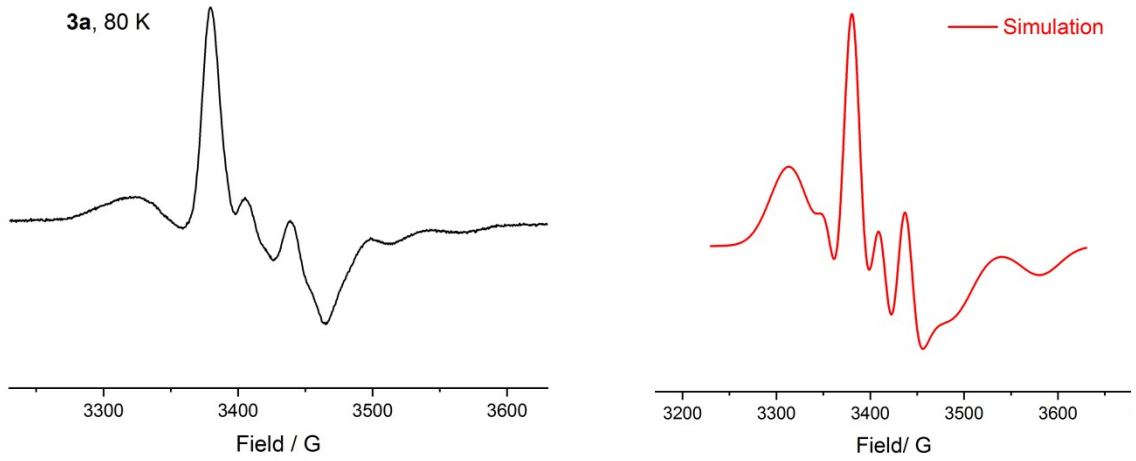


Figure S23. Experimental and simulated EPR spectrum of compound **3a** (1 mM THF solution) at 80 K. Microwave freq. 9.628 GHz, power = 2 mW, mod. freq. 100 KHz.

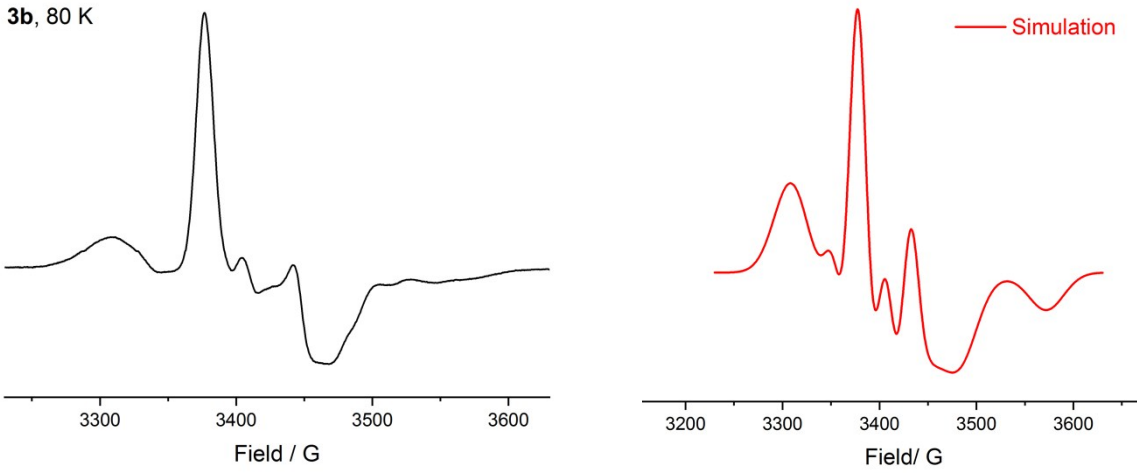


Figure S24. Experimental and simulated EPR spectrum of compound **3b** (1 mM THF solution) at 80 K. Microwave freq. 9.628 GHz, power = 2 mW, mod. freq. 100 KHz.

Simulation parameters (g-values, g_x, g_y and g_z; linewidth parameters l_x, l_y and l_z [MHz] and hyperfine coupling constants A_x, A_y and A_z [MHz]) used in the EPR simulations at 80 K, and comparison to DFT calculations (M06-2X/def2TZVP).

	Simulation		DFT	
	3a	**3b**	**3a**	**3b**
g_x	2.0237	2.0566	2.0238	2.0242
g_y	2.0064	2.0058	2.0028	2.0028
g_z	1.9960	2.0000	1.9964	1.9959
l_x	49	48		
l_y	87	101		
l_z	137	117		
A_x	-76	-72	-78	-83
A_y	2	4	-70	-75
A_z	253	248	149	158

Single Crystal X-Ray Crystallographic Details

The single crystal data were examined on a Rigaku Supernova diffractometer using either MoKα (λ = 0.71073 Å) or CuKα (λ = 1.54184 Å) radiation. The crystals were kept at 100.0(1) K during data collection. Using Olex2[4], the structure was solved with the ShelXT[5] structure solution program using Intrinsic Phasing and refined with the ShelXL[6] refinement package using Least Squares minimization. Hydrogen atoms were taken into account using a riding model. Details of the X-ray investigation are given in Table T1 and T2. CCDC 1966689-1966694 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/conts/retrieving.html.

Table S1. Crystal data and structure refinement for compounds **2a**, **2b**, and **3a**.

	2a	**2b**	**3a**
Empirical formula	$C_{54}H_{72}AsN_3$	$C_{57}H_{76}AsN_3$	$C_{54}H_{72}AsCl_4GaN_3$
Formula weight	838.06	878.12	1049.58
Temperature/K	100.0(1)	100.0(1)	100.0(1)
Crystal system	monoclinic	monoclinic	triclinic
Space group	$P2_1/n$	$P2_1/c$	P-1
a/Å	12.59029(7)	18.8381(6)	11.4502(3)
b/Å	15.93625(8)	11.9051(4)	19.3524(5)
c/Å	23.78509(12)	22.8999(7)	25.1018(7)
α/°	90	90	76.229(2)
β/°	93.2310(5)	101.668(3)	89.254(2)
γ/°	90	90	88.856(2)
Volume/Å^3	4764.70(4)	5029.6(3)	5401.1(3)
Z	4	4	4
ρ_{calc}g/cm^3	1.168	1.160	1.291
μ/mm^{-1}	1.235	0.714	1.352
F(000)	1800.0	1888.0	2196.0
Crystal size/mm^3	0.301 × 0.147 × 0.108	0.229 × 0.089 × 0.026	0.153 × 0.118 × 0.029
Radiation/Å	Cu Kα (λ = 1.54184)	Mo Kα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.68 to 153.038	3.632 to 64.312	3.034 to 64.308
Index ranges	-15 ≤ h ≤ 15, -20 ≤ k ≤ 20, -29 ≤ l ≤ 29	-19 ≤ h ≤ 27, -16 ≤ k ≤ 17, -34 ≤ l ≤ 31	-16 ≤ h ≤ 16, -28 ≤ k ≤ 28, -37 ≤ l ≤ 37
Reflections collected	132664	41417	96628
Independent reflections	9986 [R_{int} = 0.0523, R_{sigma} = 0.0195]	15892 [R_{int} = 0.0567, R_{sigma} = 0.0866]	34476 [R_{int} = 0.0596, R_{sigma} = 0.0807]
Reflections with *I* > 2σ(*I*)	9089	10560	23488
Data/restraints/parameters	9986/0/811	15892/0/564	34476/0/1167
Goodness-of-fit on F^2	1.026	1.036	1.041
Final R indexes [*I* > 2σ(*I*)]	R_1 = 0.0269, wR_2 = 0.0677	R_1 = 0.0554, wR_2 = 0.1071	R_1 = 0.0550, wR_2 = 0.1135
Final R indexes [all data]	R_1 = 0.0307, wR_2 = 0.0705	R_1 = 0.1008, wR_2 = 0.1247	R_1 = 0.0956, wR_2 = 0.1294
Largest diff. peak/hole / e Å^{-3}	0.39/-0.41	0.45/-0.52	1.39/-0.69
CCDC	1966689	1966690	1966691

Table S2. Crystal data and structure refinement for compounds **3b**, **4a**, and **4b**.

	3b	**4a**	**4b**
Empirical formula	$C_{57}H_{76}AsCl_4GaN_3$	$C_{54}H_{72}AsCl_8Ga_2N_3$	$C_{57}H_{76}AsCl_8Ga_2N_3$
Formula weight	1089.64	1261.10	1301.16
Temperature/K	100.0(1)	100.0(1)	100.0(1)
Crystal system	monoclinic	orthorhombic	triclinic
Space group	$P2_1/n$	Pbca	P-1
a/Å	12.6066(3)	18.8893(4)	13.7117(5)
b/Å	23.8366(5)	26.1136(4)	24.2939(7)
c/Å	18.7085(4)	24.2536(4)	24.8610(8)
α/°	90	90	100.452(2)
β/°	98.410(2)	90	98.045(3)
γ/°	90	90	98.408(3)
Volume/Å^3	5561.4(2)	11963.5(4)	7937.7(5)
Z	4	8	4
ρ_{calc}g/cm^3	1.301	1.400	1.089
μ/mm^{-1}	1.316	5.283	1.391
F(000)	2284.0	5184.0	2680.0
Crystal size/mm^3	0.435 × 0.272 × 0.169	0.244 × 0.169 × 0.045	0.167 × 0.11 × 0.043
Radiation/Å	MoKα (λ = 0.71073)	Cu Kα (λ = 1.54184)	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.418 to 64.3	6.77 to 136.482	3.048 to 50.7
Index ranges	-18 ≤ h ≤ 18, -33 ≤ k ≤ 29, -26 ≤ l ≤ 27	-22 ≤ h ≤ 22, -30 ≤ k ≤ 31, -29 ≤ l ≤ 29	-16 ≤ h ≤ 16, -29 ≤ k ≤ 29, -29 ≤ l ≤ 29
Reflections collected	58501	141043	97309
Independent reflections	17861 [R_{int} = 0.0446, R_{sigma} = 0.0514]	10879 [R_{int} = 0.1217, R_{sigma} = 0.0466]	29076 [R_{int} = 0.0664, R_{sigma} = 0.0755]
Reflections with *I* > 2σ(*I*)	13268	8619	19032
Data/restraints/parameters	17861/0/609	10879/92/661	29076/0/1344
Goodness-of-fit on F^2	1.011	1.087	1.012
Final R indexes [*I* > 2σ(*I*)]	R_1 = 0.0403, wR_2 = 0.0850	R_1 = 0.0676, wR_2 = 0.1669	R_1 = 0.0498, wR_2 = 0.1177
Final R indexes [all data]	R_1 = 0.0661, wR_2 = 0.0949	R_1 = 0.0850, wR_2 = 0.1792	R_1 = 0.0829, wR_2 = 0.1308
Largest diff. peak/hole / e Å^{-3}	0.71/-0.61	1.25/-0.73	0.87/-0.47
CCDC	1966692	1966693	1966694

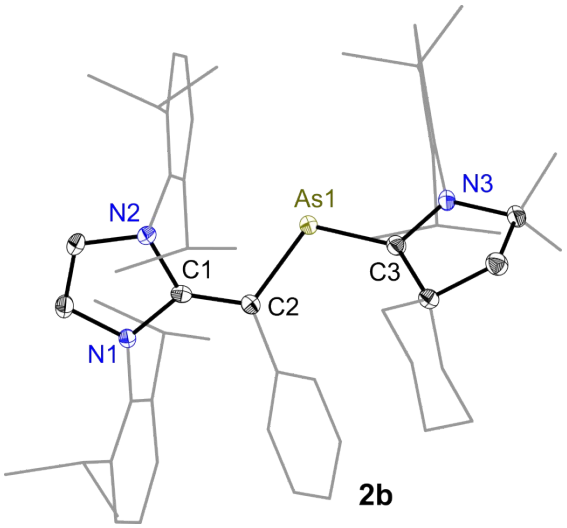


Figure S25. Solid-state molecular structures of 2-arsa-1,3-butadienes **2b**. Hydrogen atoms have been omitted for clarity. Selected bond lengths (Å) and bond angles (º): C2–As1 1.947(2), As1–C3 1.861(2), C1–C2 1.374(3), N1–C1 1.406(3), N2–C1 1.419(3), N3–C3 1.379(3); C2–As1–C3 109.0(1), C1–C2–As1 117.7(2), C2–C1–N1 128.5(2), C2–C1–N2 128.4(2), As1–C3–N3 115.9(1).

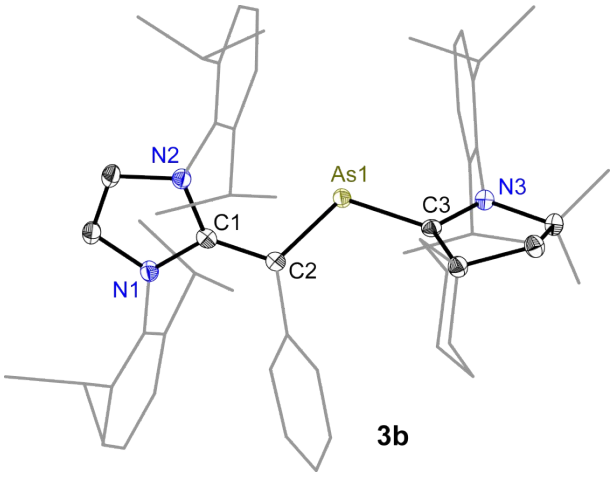


Figure S26. Solid-state molecular structures of radical cation **3b**. Hydrogen atoms, second molecules, and the counter anions $GaCl_4$ have been omitted for clarity. Selected bond lengths (Å) and bond angles (º): C2–As1 1.887(2), As1–C3 1.929(2), C1–C2 1.419(2), N1–C1 1.379(2), N2–C1 1.381(2), N3–C3 1.335(2); C2–As1–C3 109.2(1), C1–C2–As1 115.7(1), C2–C1–N1 128.6(2), C2–C1–N2 126.9(2), As1–C3–N3 115.2(1).

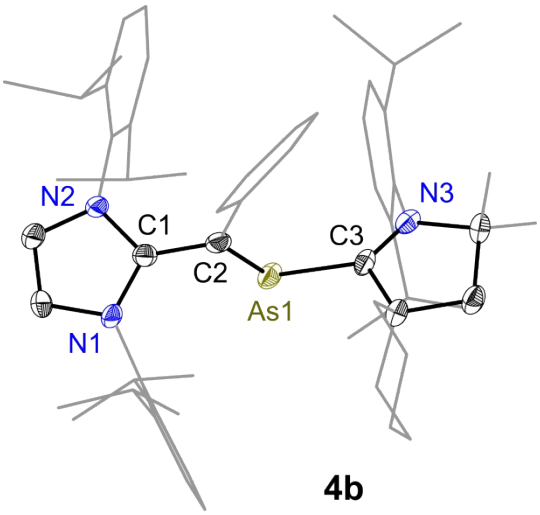


Figure S27. Solid-state molecular structures of dication **4b**. Hydrogen atoms and the counter anions $GaCl_4$ have been omitted for clarity. Selected bond lengths (Å) and bond angles (º): C2–As1 1.826(4), C3–As1 2.001(4), C1–C2 1.459(5), N1–C1 1.357(5), N2–C1 1.345(4), N3–C3 1.287(5); C2–As1–C3 101.9(2), C1–C2–As1 116.3(3), C2–C1–N1 128.0(3), C2–C1–N2 124.8(3), As1–C3–N3 122.7(3).

Computational Details

All geometries were optimized with the Gaussian 16 program suite[7] using the DFT functional M06-2X[8] in combination with the Ahlrich's def2-SVP[9] basis function as implemented. The stationary points were located with the Berny algorithm using redundant internal coordinates. Analytical Hessians were computed to determine the nature of stationary points (zero imaginary frequencies for minima).[10] The electronic energies were improved by single point calculations at the M06-2X/def2-TZVPP level of theory.

The Wiberg Bond Indices (WBI)[11] and NPA[12] atomic partial charges were calculated at the M06-2X/def2-TZVPP//M06-2X/def2-SVP level of theory using the NBO 3.1 interface of Gaussian.[13]

Time-dependent density functional theory (Full-TDDFT) was employed to calculate excitation energies as implemented in ORCA 4.0.1.[14] We used the functional M06-2X in combination the def2-SVP basis sets. The solvent (THF) was described by the conductor-like polarizable continuum model, CPCM.[15]

Table S3. Electronic energies of selected molecular orbitals of compounds **2a-b**, **3a-b**, and **4a-b** calculated at M06-2X/def2-TZVPP//M06-2X/def2-SVP level of theory. For the radical cations **3a** and **3b**, the value for both (α/β) spin orbitals are given

orbital	energy / eV					
	2a	**2b**	**3a**	**3b**	**4a**	**4b**
L+1	+0.29	+0.29	−2.49/−2.51	−2.46/−2.52	−5.97	−5.94
L	+0.09	+0.06	−3.10/−4.57	−3.14/−4.53	−7.89	−7.82
S/ H	−4.89	−4.89	−7.98/−9.28	−7.94/−9.24	−12.72	−12.71
S−1/ H−1	−6.28	−6.25	−9.88/−9.94	−9.84/−9.90	−12.76	−12.73
S−2/ H−2	−6.94	−6.92	−1.01/−10.24	−9.98/−10.24	−12.87	−12.83
S−3/ H−3	−7.61	−7.65	−10.25/−10.30	−10.25/−10.28	−12.95	−12.92
S−4// H−4	−7.76	−7.74	−10.33/−10.40	−10.31/−10.38	−13.03	−12.99
SOMO-LUMO or HOMO-LUMO gap	4.98	4.95	4.88/4.71	4.80/4.71	4.83	4.89
L = lowest unoccupied molecular orbital (LUMO); S = singly occupied molecular orbital (SOMO); H = highest occupied molecular orbital (HOMO)						

Table S4. Wiberg bond indices as well as natural population analysis (NPA) atomic charges of compounds **2a-b**, **3a-b**, and **4a-b** calculated at M06-2X/def2-TZVPP//def2-SVP level of theory.

bond	Wiberg bond indices					
	2a	**2b**	**3a**	**3b**	**4a**	**4b**
As–C(C–Ph)	0.90	0.90	1.13	1.13	1.56	1.57
C(C–Ph)–C(IPr)$_{ipso}$	1.53	1.53	1.25	1.25	1.09	1.09
C(IPr)$_{ipso}$–N(IPr)$_{cis}$[a]	1.07	1.07	1.18	1.18	1.25	1.25
C(IPr)$_{ipso}$–N(IPr)$_{trans}$[a]	1.06	1.06	1.17	1.17	1.25	1.25
N(IPr)$_{cis}$–C(IPr)$_{cis}$	1.06	1.06	1.11	1.10	1.16	1.16
N(IPr)$_{trans}$–C(IPr)$_{trans}$	1.07	1.07	1.12	1.12	1.17	1.17
C(IPr)cis–C(IPr)$_{trans}$	1.73	1.73	1.66	1.66	1.59	1.59
As–C(pyrollidine)	1.50	1.49	1.11	1.09	0.87	0.87
C(pyrollidine)$_{ipso}$–N(pyrollidine)	1.14	1.15	1.37	1.37	1.62	1.61
C(pyrollidine)$_{ipso}$–C(Me$_2$)$^{\beta}$	0.96	0.97	0.97	0.98	0.98	1.00
atom	**NPA atomic charge**					
	2a	**2b**	**3a**	**3b**	**4a**	**4b**
As	+0.51	+0.50	+0.69	+0.69	+0.94	+0.94
C(C–Ph)	−0.57	−0,57	−0.55	−0.55	−0.45	−0.46
C(IPr)$_{ipso}$	+0.42	+0.42	+0.45	+0.45	+0.41	+0.41
N(IPr)$_{cis}$	−0.45	−0.45	−0.37	−0.37	−0.32	−0.32
N(IPr)$_{trans}$	−0.45	−0.45	−0.37	−0.37	−0.31	−0.32
C(IPr)$_{cis}$	−0.09	−0.09	−0.06	−0.06	−0.03	−0.04
C(IPr)$_{trans}$	−0.08	−0.08	−0.05	−0.05	−0.03	−0.03
C(C=As)	−0.05	−0.04	−0.09	+0.10	+0.24	+0.25
N(N–C=As)	−0.50	−0.50	−0.41	−0.41	−0.35	−0.35
C(C–C=As)$^{\beta}$	−0.14	−0.13	−0.15	−0.14	−0.16	−0.15

[a] This nomenclature is chosen to distinguish between the different C–N and N–C bonds within the IPr substituents. Herein, *cis* means that the nitrogen atom involved in the above-mentioned bonds is approximately *cis*-oriented with respect to the arsenic atom.

Table S5. Wavelength (λ), oscillator strength (f) and main assignment of the TD-PCM(thf)/M06-2X/def2-SVP results for compound **2a**; threshold for printing excitations was chosen to be $f \geq 0.06$.

state no.	**λ / nm**	***f***	**Assignment**
1	413.0	0.1322	H → L (c = 0.9242)
2	383.6	0.1983	H → L+1 (c = 0.8349)
15	247.4	0.1043	H → L+11 (c = 0.2514)
36	208.6	0.0909	H−2 → L+7 (c = 0.2177)
45	200.7	0.0726	H−5 → L (c = 0.2583)

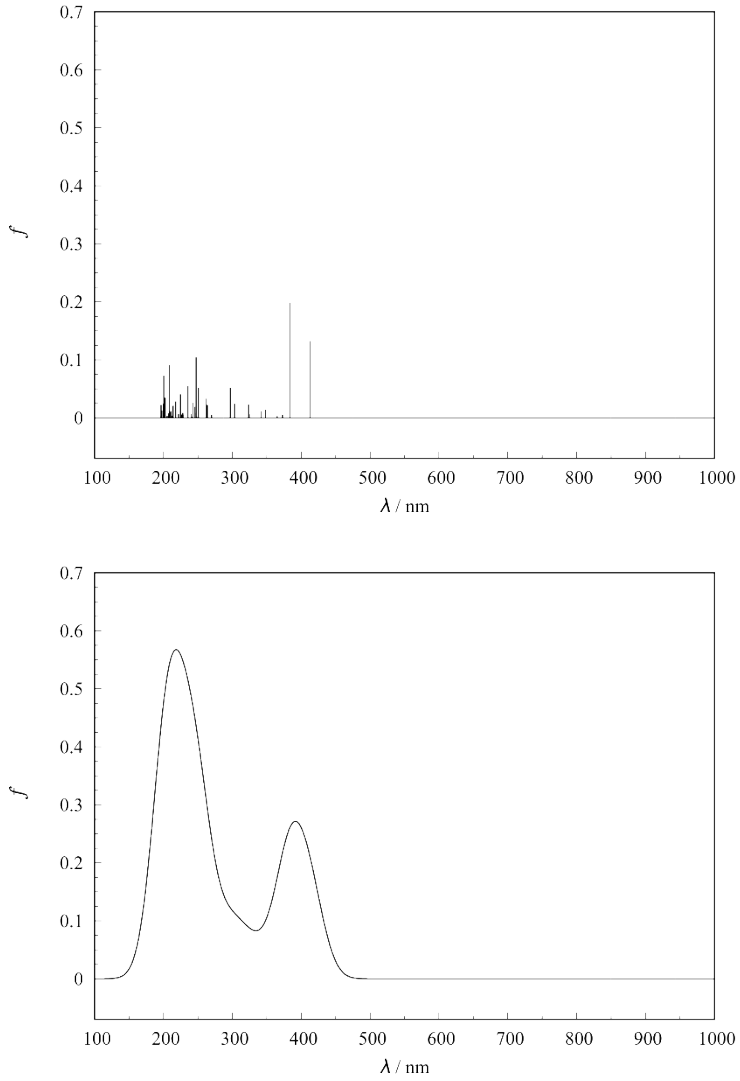


Figure S28. UV-visible spectrum (lines: top; Gaussian line broadening with a full width at half maximum (fwhm) of 50 cm^{-1}: bottom) of **2a** calculated at TD-PCM(thf)/M06-2X/def2-SVP.

Table S6. Wavelength (λ), oscillator strength (f) and main assignment of the TD-PCM(thf)/M06-2X/def2-SVP results for compound **2b**; threshold for printing excitations was chosen to be $f \geq 0.06$.

state no.	**λ / nm**	***f***	**Assignment**
1	418.1	0.1422	H → L (c = 0.9347)
2	384.1	0.1666	H → L+1 (c = 0.8349)
15	249.3	0.0999	H → L+10 (c = 0.2537)
45	202.1	0.0742	H−2 → L+6 (c = 0.2490)

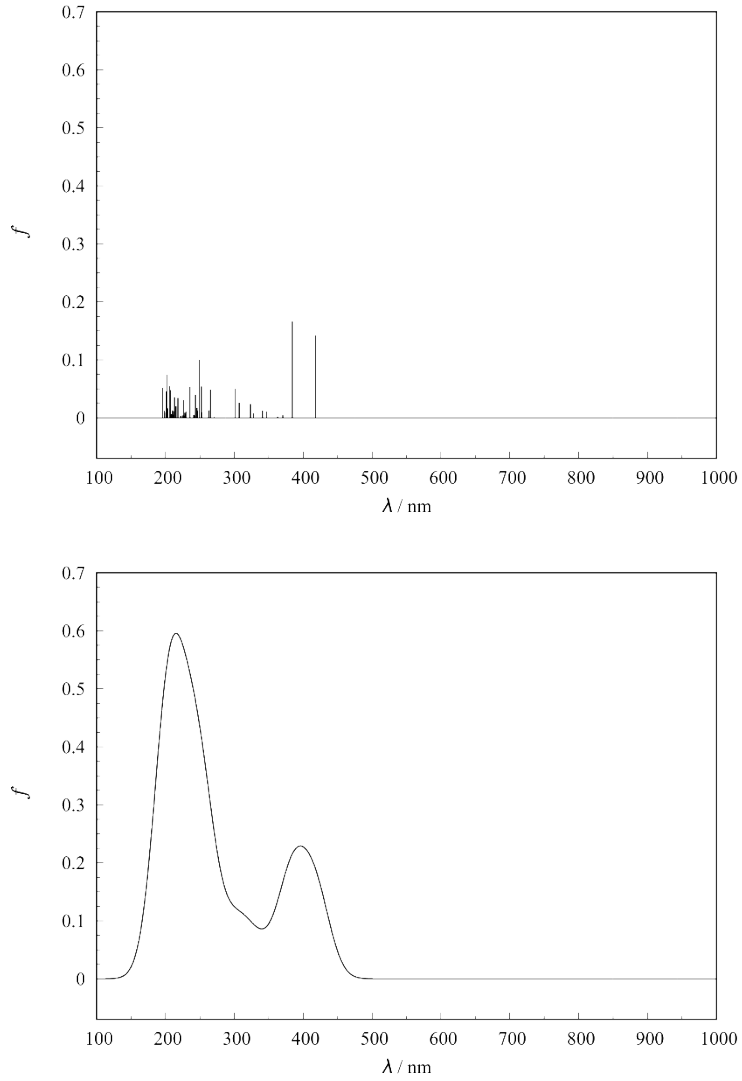


Figure S29. UV-visible spectrum (lines: top; Gaussian line broadening with a full width at half maximum (fwhm) of 50 cm^{-1}: bottom) of **2b** calculated at TD-PCM(thf)/M06-2X/def2-SVP.

Table S7. Wavelength (λ), oscillator strength (f) and main assignment of the TD-PCM(thf)/M06-2X/def2-SVP results for compound **3a**; threshold for printing excitations was chosen to be $f \geq 0.03$.

state no.	λ / nm	f	Assignment
1	681.3	0.1218	S–1 → S (c = 0.9139)
2	557.4	0.1443	S → L (c = 0.8850)
4	400.4	0.0363	S → L+1 (c = 0.7513)
22	296.1	0.0378	S−8 → S (c = 0.5789)
41	250.7	0.0484	S → L+12 (c = 0.2437)
44	240.5	0.0388	S–1 → L+1 (c = 0.3335)

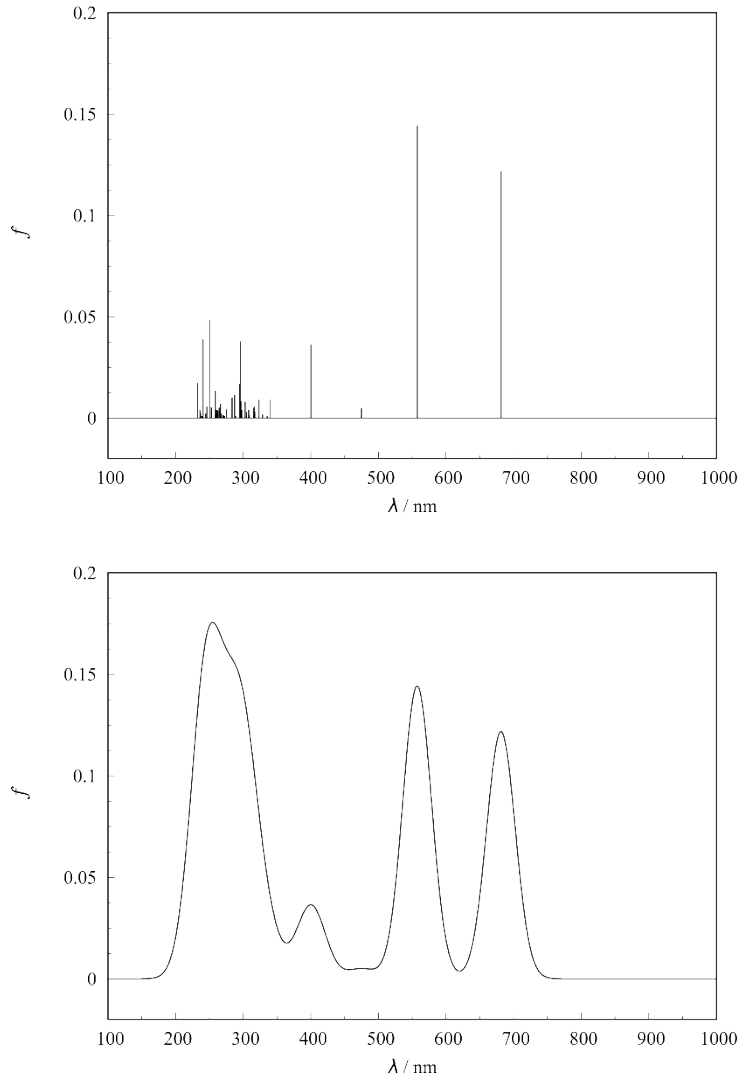


Figure S30. UV-visible spectrum (lines: top; Gaussian line broadening with a full width at half maximum (fwhm) of 50 cm^{-1}: bottom) of **3a** calculated at TD-PCM(thf)/M06-2X/def2-SVP.

Table S8. Wavelength (λ), oscillator strength (f) and main assignment of the TD-PCM(thf)/M06-2X/def2-SVP results for compound **3b**; threshold for printing excitations was chosen to be $f \geq 0.03$.

state no.	**λ / nm**	***f***	**Assignment**
1	684.8	0.1215	S−1 → S (c = 0.9151)
2	574.1	0.1335	S → L (c = 0.8901)
4	397.8	0.0371	S → L+1 (c = 0.7737)
41	252.5	0.0540	S → L+12 (c = 0.2122)
44	240.7	0.0313	S−1 → L+1 (c = 0.2839)

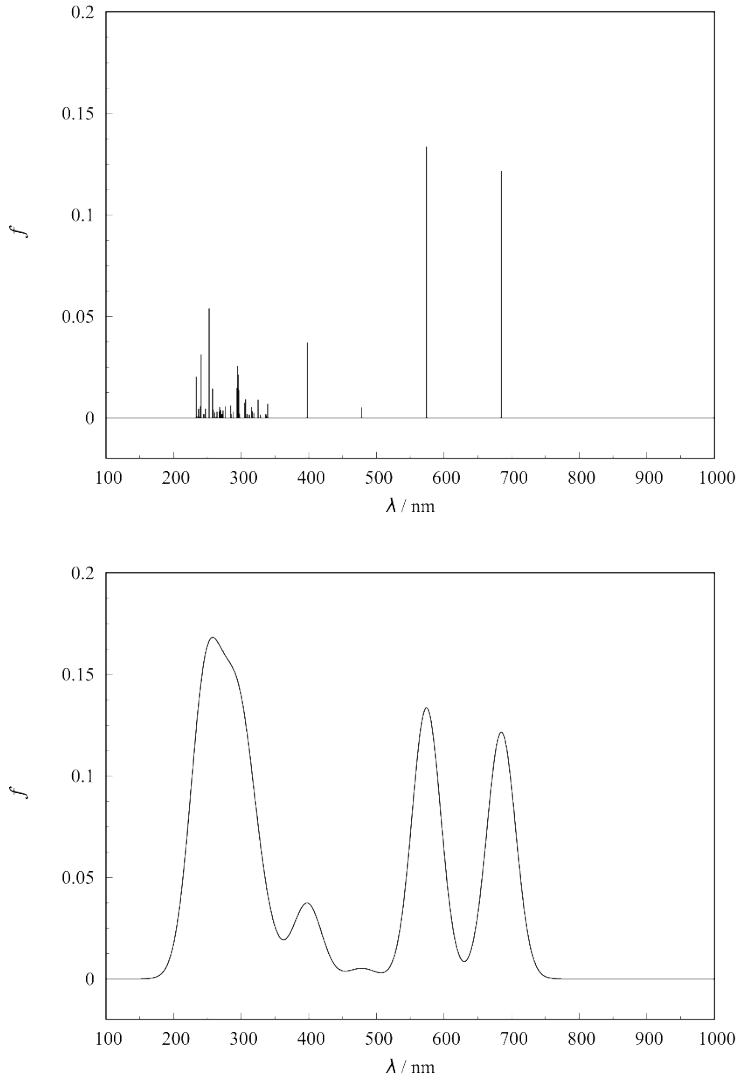


Figure S31. UV-visible spectrum (lines: top; Gaussian line broadening with a full width at half maximum (fwhm) of 50 cm^{-1}: bottom) of **3b** calculated at TD-PCM(thf)/M06-2X/def2-SVP.

Table S9. Wavelength (λ), oscillator strength (f) and main assignment of the TD-PCM(thf)/M06-2X/def2-SVP results for compound **4a**; threshold for printing excitations was chosen to be $f \geq 0.04$.

state no.	**λ / nm**	***f***	**Assignment**
2	419.2	0.1969	H → L (c = 0.6464)
6	357.2	0.0569	H−6 → L (c = 0.6671)
8	326.9	0.0992	H−7 → L (c = 0.9148)
12	261.5	0.0429	H → L+1 (c = 0.3593)
23	225.8	0.0898	H → L+2 (c = 0.3137)
46	201.3	0.0677	H−6 → L+5 (c = 0.0514) H → L+8 (c = 0.0515)

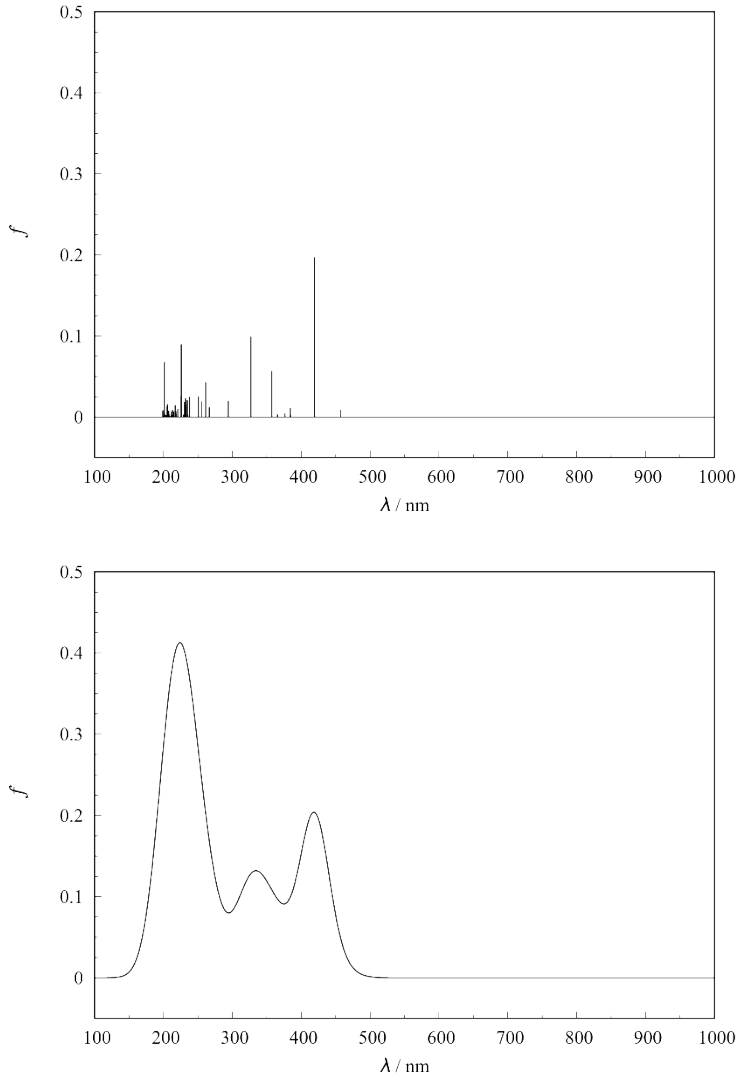


Figure S32. UV-visible spectrum (lines: top; Gaussian line broadening with a full width at half maximum (fwhm) of 50 cm^{-1}: bottom) of **4a** calculated at TD-PCM(thf)/M06-2X/def2-SVP.

Table S10. Wavelength (λ), oscillator strength (f) and main assignment of the TD-PCM(thf)/M06-2X/def2-SVP results for compound **4b**; threshold for printing excitations was chosen to be $f \geq 0.04$.

state no.	**λ / nm**	***f***	**Assignment**
2	416.3	0.2042	H → L (c = 0.7401)
8	325.7	0.0709	H−7 → L (c = 0.8583)
25	225.5	0.1265	H → L+2 (c = 0.4543)
49	201.5	0.0721	H−9 → L (c = 0.0761)

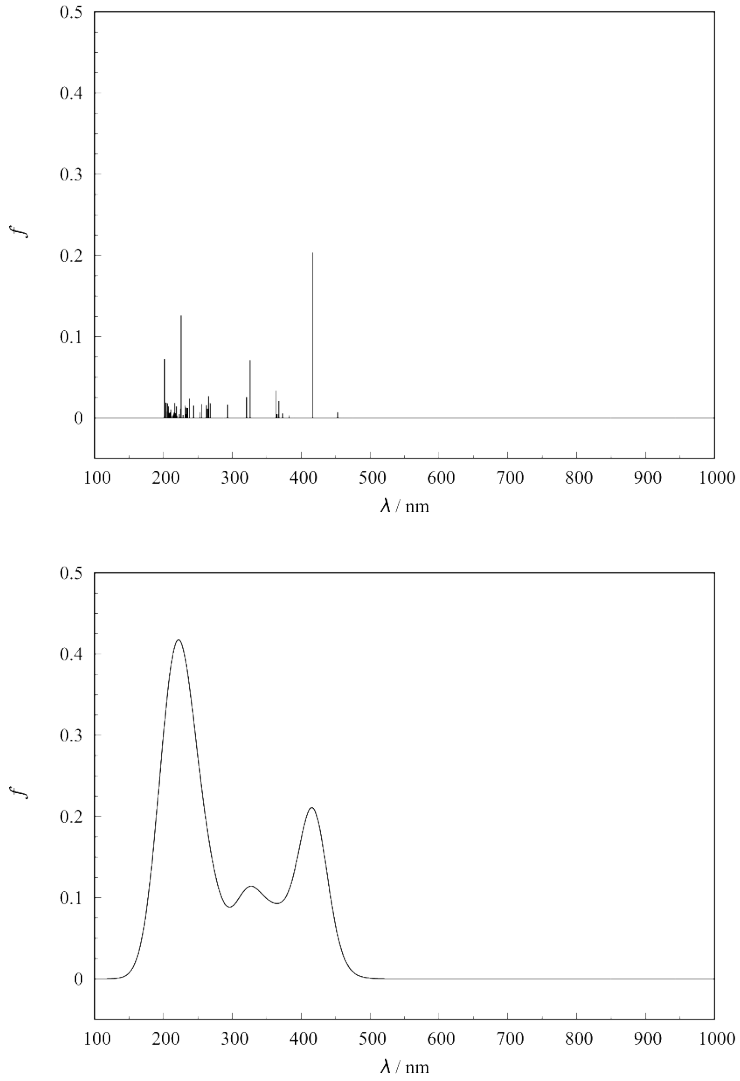
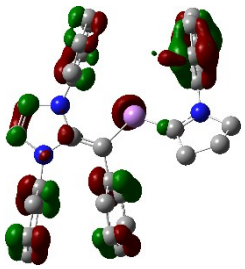


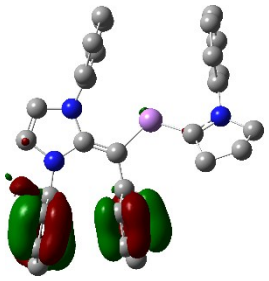
Figure S33. UV-visible spectrum (lines: top; Gaussian line broadening with a full width at half maximum (fwhm) of 50 cm^{-1}: bottom) of **4b** calculated at TD-PCM(thf)/M06-2X/def2-SVP.

Table S11. Calculated *g*-factor and hyperfine coupling constants (*A* in MHz), Löwdin and Mulliken (in parenthesis) spin densities for the arsabutadiene radical cations **3a** and **3b** calculated at the TPSS/decon-def2-TZVP//M06-2X/def2-SVP level of theory.

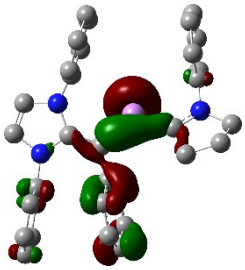
	3a	**3b**
g-factor	2.0060857	2.0061639
$A_{iso}(As)$	38.6512	41.9547
$A_{iso}(N_{IPr\_cis})$	3.2196	3.2070
$A_{iso}(N_{IPr\_trans})$	4.6039	4.5099
$A_{iso}(N_{pyrollidine})$	6.8914	6.8262
$A_{iso}(H_{Ph\text{-}ortho})$	−1.2318	−1.0922
$A_{iso}(H_{Ph\text{-}ortho})$	−1.3052	−1.2064
$A_{iso}(H_{Ph\text{-}para})$	−0.6674	−0.5516
$A_{iso}(H_{IPr})$	−2.4688	−2.4866
$A_{iso}(H_{IPr})$	−1.7101	−1.7446
$\rho_{spin}(As)$	0.20(0.21)	0.21(0.23)
$\rho_{spin}(C_{vinylic})$	0.22(0.26)	0.21(0.25)
$\rho_{spin}(C_{carb\text{-}ipso})$	0.04(0.02)	0.04(0.02)
$\rho_{spin}(N_{IPr\_cis})$	0.05(0.06)	0.05(0.06)
$\rho_{spin}(N_{IPr\_trans})$	0.05(0.07)	0.05(0.06)
$\rho_{spin}(C_{IPr\_cis})$	0.04(0.04)	0.04(0.04)
$\rho_{spin}(C_{IPr\_trans})$	0.03(0.02)	0.03(0.03)
$\rho_{spin}(C_{Ph\text{-}ipso})$	0.02(0.00)	0.02(0.00)
$\rho_{spin}(C_{Ph\text{-}ortho})$	0.01(0.01)	0.01(0.01)
$\rho_{spin}(C_{Ph\text{-}ortho})$	0.01(0.02)	0.01(0.02)
$\rho_{spin}(C_{Ph\text{-}para})$	0.01(0.01)	0.01(0.01)
$\rho_{spin}(C_{pyrollidine\text{-}ipso})$	0.13(0.16)	0.13(0.16)
$\rho_{spin}(N_{pyrollidine})$	0.11(0.13)	0.11(0.13)



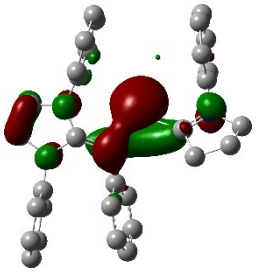
HOMO−4



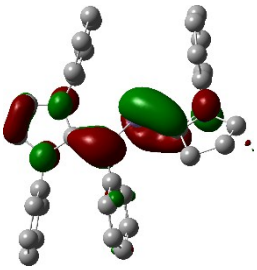
HOMO−3



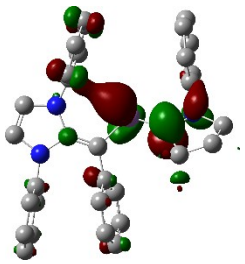
HOMO−2



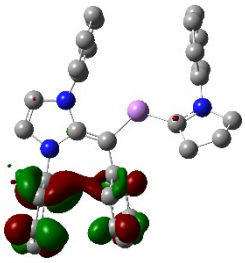
HOMO−1



HOMO



LUMO



LUMO+1

Figure S34. Selected molecular orbitals (from HOMO−4 to LUMO+1) of compound **2a**, calculated at M06-2X/def2-TZVPP//def2-SVP. The isovalue was arbitrarily chosen to be 0.04. Hydrogen atoms, methyl groups as well as *iso*-propyl groups were omitted for clarity reasons.

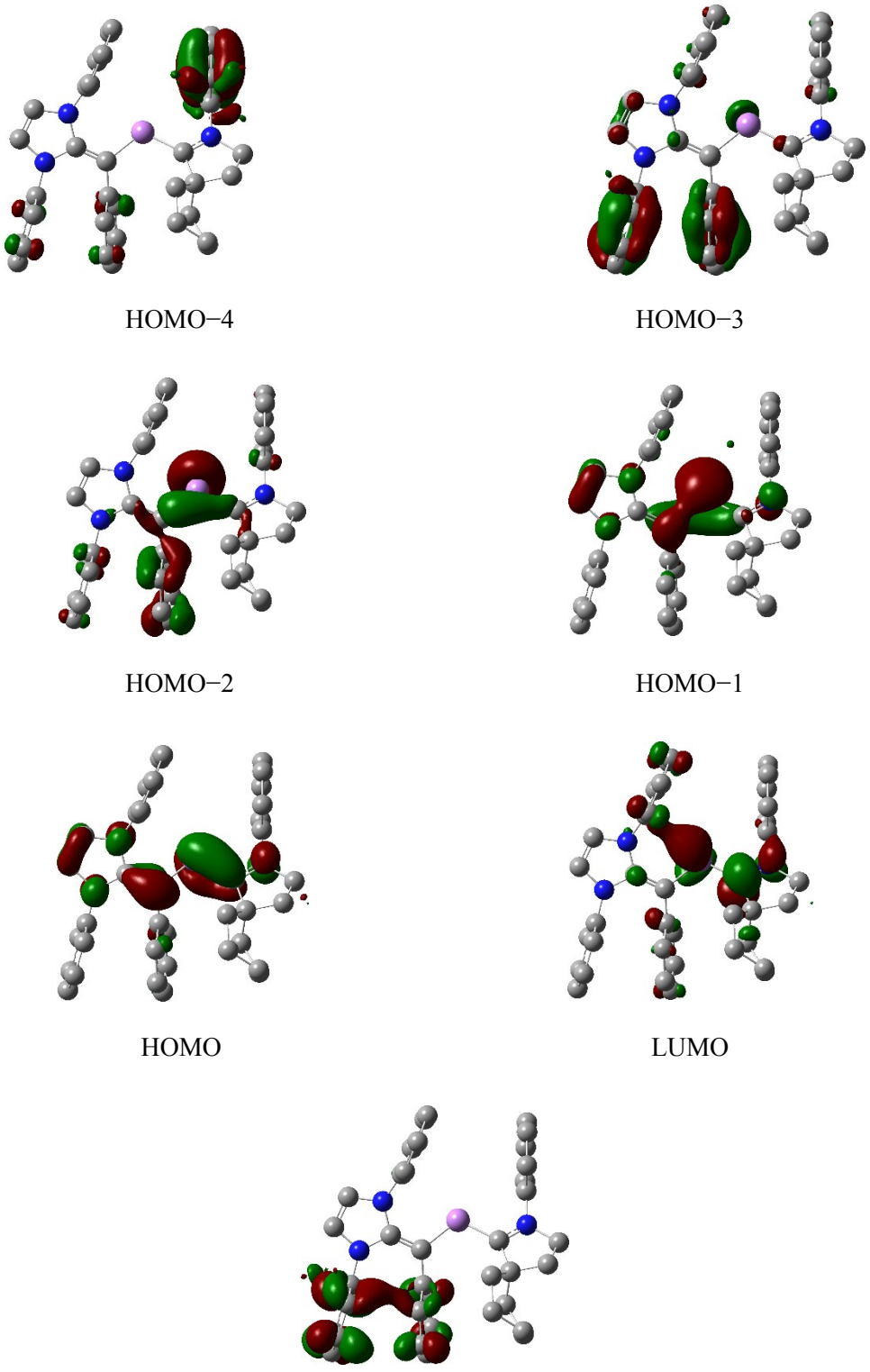
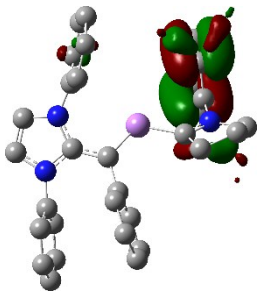
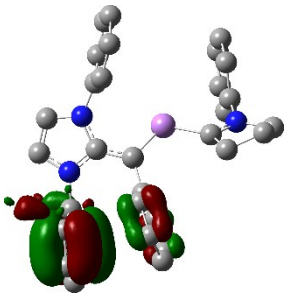


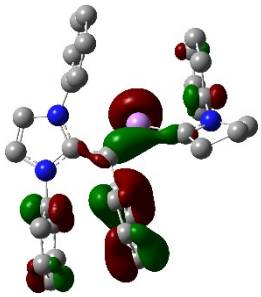
Figure S35. Selected molecular orbitals (from HOMO−4 to LUMO+1) of compound **2b**, calculated at M06-2X/def2-TZVPP//def2-SVP. The isovalue was arbitrarily chosen to be 0.04. Hydrogen atoms, methyl groups as well as *iso*-propyl groups were omitted for clarity reasons.



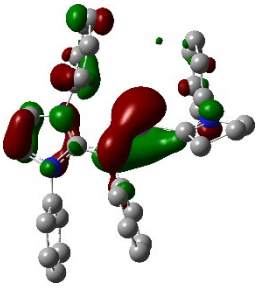
SOMO−4



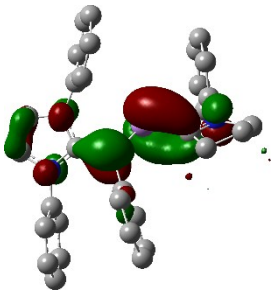
SOMO−3



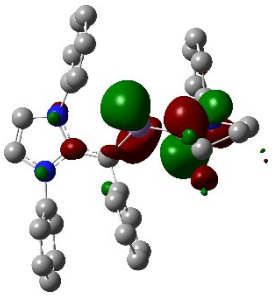
SOMO−2



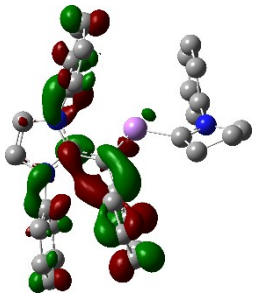
SOMO−1



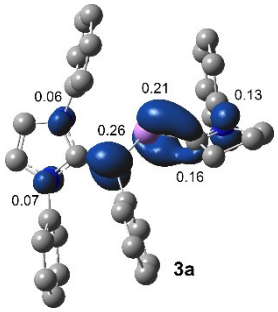
SOMO



LUMO

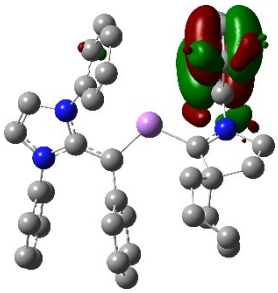


LUMO+1

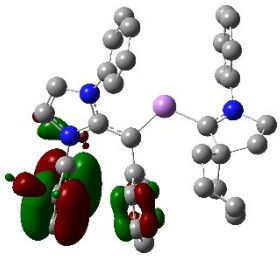


spin density

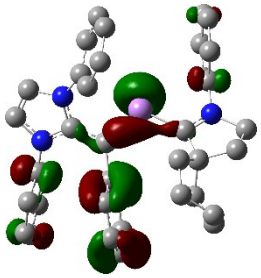
Figure S36. Selected molecular orbitals (from SOMO−4 to LUMO+1) and spin density plot of compound **3a**, calculated at M06-2X/def2-TZVPP//def2-SVP. The isovalue was arbitrarily chosen to be 0.04 for molecular orbitals and 0.004 for spin density. Hydrogen atoms, methyl groups as well as *iso*-propyl groups were omitted for clarity reasons.



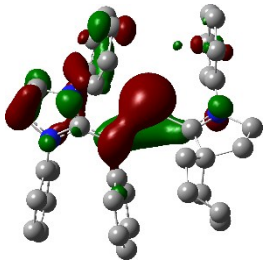
SOMO−4



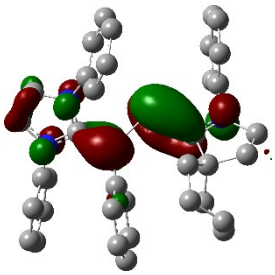
SOMO−3



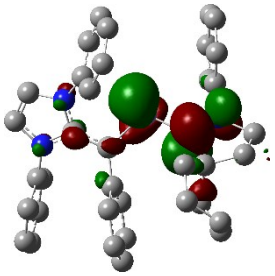
SOMO−2



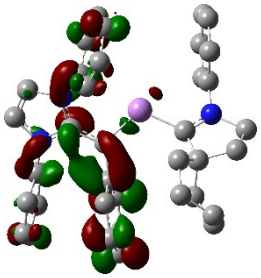
SOMO−1



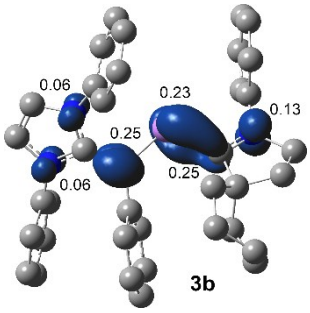
SOMO



LUMO

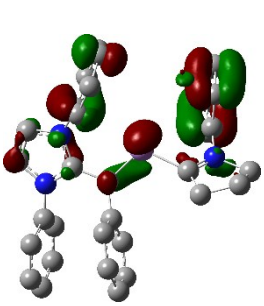


LUMO+1

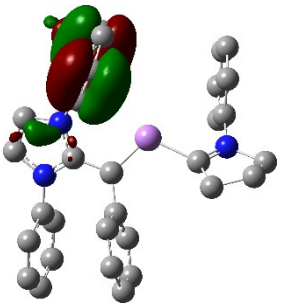


spin density

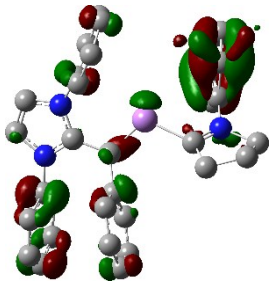
Figure S37. Selected molecular orbitals (from SOMO−4 to LUMO+1) and spin density plot of compound **3b**, calculated at M06-2X/def2-TZVPP//def2-SVP. The isovalue was arbitrarily chosen to be 0.04 for molecular orbitals and 0.004 for spin density. Hydrogen atoms, methyl groups as well as *iso*-propyl groups were omitted for clarity reasons.



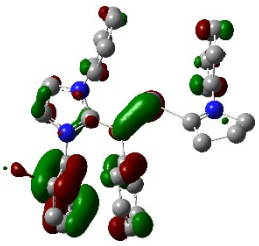
HOMO−4



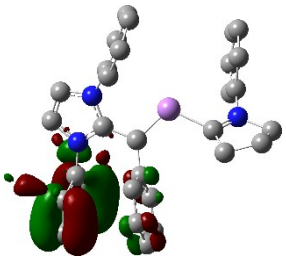
HOMO−3



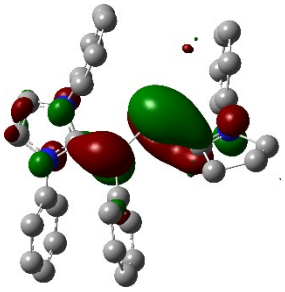
HOMO−2



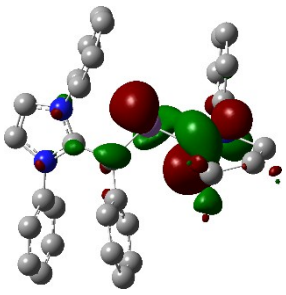
HOMO−1



HOMO



LUMO



LUMO+1

Figure S38. Selected molecular orbitals (from HOMO−4 to LUMO+1) of compound **4a**, calculated at M06-2X/def2-TZVPP//def2-SVP. The isovalue was arbitrarily chosen to be 0.04. Hydrogen atoms, methyl groups as well as *iso*-propyl groups were omitted for clarity reasons.

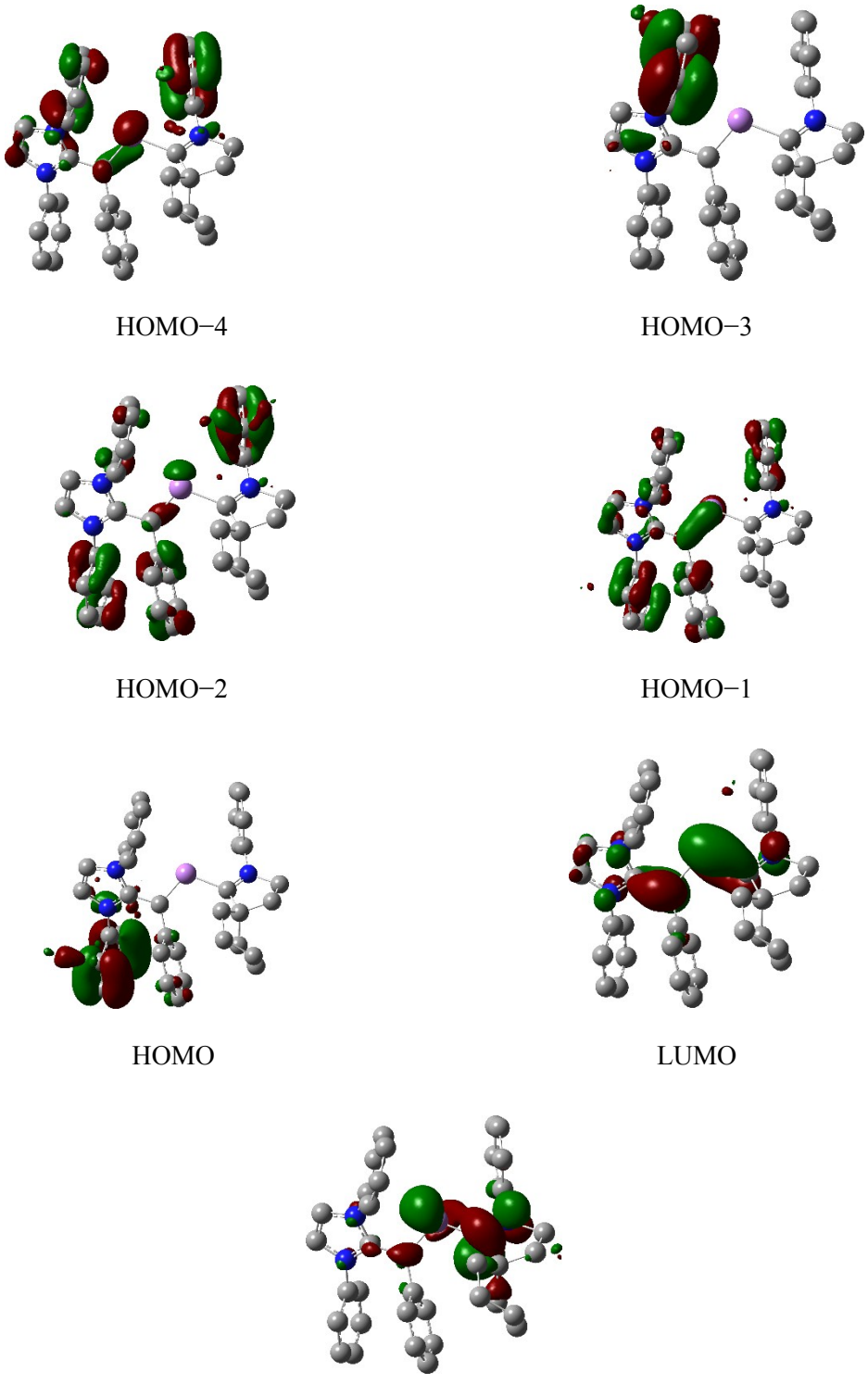


Figure S39. Selected molecular orbitals (from HOMO−4 to LUMO+1) of compound **4b**, calculated at M06-2X/def2-TZVPP//def2-SVP. The isovalue was arbitrarily chosen to be 0.04. Hydrogen atoms, methyl groups as well as *iso*-propyl groups were omitted for clarity reasons.

2a ν_{min} = 14 cm^{-1} *E* = -4498.2889419

C	1.833868	0.687798	0.395966
C	1.025734	-0.350871	-0.035483
C	1.612818	-1.700348	-0.249997
As	-0.886967	-0.207866	0.355433
N	1.453771	1.989428	0.775958
C	2.543001	2.662454	1.342322
C	3.605651	1.848026	1.296819
N	3.205548	0.650408	0.709563
C	0.388259	2.833122	0.309299
C	-0.638302	3.182541	1.205505
C	-1.529300	4.189258	0.821461
C	-1.397060	4.833646	-0.404016
C	0.536111	3.468721	-0.939931
C	-0.382528	4.465591	-1.282061
C	1.655063	3.080482	-1.892101
H	-0.290984	4.975492	-2.242188
H	-2.095762	5.624837	-0.682092
C	-0.755821	2.538270	2.575814
H	-2.332689	4.479281	1.501067
H	2.440155	3.684919	1.689198
H	4.625861	1.981523	1.641753
C	4.167672	-0.394064	0.533809
C	4.396921	-1.320316	1.561966
C	5.371903	-2.303993	1.332919
C	6.122885	-2.330413	0.167920
C	5.904973	-1.373424	-0.821069
C	4.917433	-0.403253	-0.664914
C	4.629117	0.598243	-1.775101
H	6.495410	-1.404476	-1.737309
H	6.880070	-3.102818	0.024019
C	3.762704	-1.321828	2.953529
H	5.545617	-3.056306	2.106413
C	-0.189864	3.460212	3.662413
H	0.870563	3.691290	3.487575
H	-0.274316	2.983966	4.650617
H	-0.744487	4.411094	3.693320
H	-0.147482	1.622458	2.558637
C	-2.196219	2.135884	2.893767
H	-2.839184	3.015381	3.056269
H	-2.226599	1.532003	3.813531
H	-2.626022	1.538791	2.077532
H	2.468137	2.649086	-1.286897
C	2.242633	4.272694	-2.647955
C	1.167643	1.999265	-2.863234
H	0.774166	1.131734	-2.315269
H	1.989704	1.660449	-3.514441
H	0.364618	2.396444	-3.504745
H	2.551493	5.073603	-1.960749
H	1.524194	4.694290	-3.366747
H	3.123787	3.952793	-3.223312
C	4.915761	0.040675	-3.171288
C	5.401276	1.909374	-1.579622
H	3.552734	0.829210	-1.724802
H	5.996958	-0.054535	-3.353112
H	4.518548	0.724413	-3.935768
H	4.459097	-0.948517	-3.321495
H	6.484954	1.714967	-1.568782
H	5.130890	2.411033	-0.641762
H	5.187583	2.604511	-2.405912
C	2.430227	-0.603734	3.185776
C	4.796920	-0.801076	3.964888
H	3.589861	-2.388438	3.176341
H	5.015556	0.260225	3.768491
H	5.743158	-1.356772	3.908683
H	4.405838	-0.881033	4.989941
H	2.543811	0.490320	3.191177
H	2.051117	-0.896150	4.176395
H	1.669092	-0.864966	2.442198
C	-1.843239	-1.303087	-0.797000
N	-3.194656	-1.466440	-0.567713
C	-1.470553	-2.122022	-2.043800
C	-0.763123	-3.456823	-1.702905
C	-0.605811	-1.308154	-3.009194
C	-2.856902	-2.378105	-2.679979
C	-3.851295	-2.420459	-1.517999
C	-5.252389	-1.971066	-1.917060

C	-3.963164	-3.846502	-0.960231
H	-2.873694	-3.299175	-3.279647
H	-3.115531	-1.542445	-3.349008
H	0.325338	-3.355213	-1.763905
H	-1.066031	-4.235343	-2.419333
H	-0.995657	-3.807060	-0.688880
H	0.360759	-1.061242	-2.554889
H	-1.106551	-0.367925	-3.286824
H	-0.420527	-1.893650	-3.924047
C	-3.946279	-0.513491	0.205008
H	-4.403497	-4.493493	-1.732863
H	-4.616713	-3.879334	-0.081047
H	-2.989553	-4.265204	-0.685664
H	-5.244011	-0.990626	-2.401433
H	-5.918414	-1.924165	-1.042574
H	-5.668614	-2.699339	-2.627432
C	-4.353986	-0.764788	1.533748
C	-5.117678	0.217369	2.188141
C	-5.450078	1.419415	1.588073
C	-5.008438	1.673525	0.294456
C	-4.263516	0.730633	-0.413957
C	-3.845970	1.101982	-1.832467
H	-6.035476	2.163715	2.130195
H	-5.251507	2.625099	-0.182470
C	-4.097163	-2.008707	2.387488
H	-5.437255	0.022604	3.214945
C	-2.834782	-2.826659	2.126655
C	-5.358600	-2.883632	2.439938
H	-3.971456	-1.602019	3.404440
H	-5.642114	-3.245842	1.442217
H	-6.215149	-2.317505	2.832818
H	-5.196104	-3.757503	3.088417
H	-2.879389	-3.393079	1.192212
H	-2.703494	-3.545518	2.949340
H	-1.948377	-2.180067	2.086184
C	-2.806220	2.225200	-1.840122
C	-5.042979	1.538194	-2.692246
H	-3.386208	0.219949	-2.294247
H	-5.398685	2.533310	-2.386441
H	-5.897375	0.851534	-2.622238
H	-4.741678	1.612695	-3.747876
H	-3.246683	3.154633	-1.449898
H	-2.465821	2.424013	-2.869039
H	-1.930792	1.979050	-1.224174
C	2.431763	-1.988257	-1.351723
C	1.361099	-2.749091	0.655073
C	1.936157	-4.004992	0.489281
C	3.015377	-3.243039	-1.521455
C	2.773414	-4.259232	-0.599091
H	3.227850	-5.242580	-0.729437
H	1.727973	-4.794265	1.214380
H	2.612179	-1.200256	-2.085812
H	3.662202	-3.426811	-2.382154
H	0.691112	-2.568132	1.498283

2b ν_{min} = 10 cm^{-1} E = −4614.8816778

C	1.874012	0.962004	0.300754
C	1.042714	-0.142155	0.217384
C	1.593135	-1.503605	0.458226
As	-0.879593	0.124021	0.484142
N	1.533851	2.327948	0.282430
C	2.654898	3.108614	0.588189
C	3.699968	2.288674	0.760170
N	3.255166	0.982876	0.572114
C	0.447170	3.035497	-0.335718
C	-0.543810	3.602026	0.485391
C	-1.444916	4.497781	-0.098203
C	-1.351679	4.829982	-1.445740
C	0.548637	3.344845	-1.706958
C	-0.373516	4.246848	-2.245535
C	1.615747	2.701500	-2.577024
H	-0.316766	4.509398	-3.302803
H	-2.054871	5.542450	-1.880994
C	-0.606751	3.304103	1.973243
H	-2.222635	4.951833	0.518339
H	2.581164	4.190391	0.617120
H	4.735154	2.490046	1.016165
C	4.194999	-0.092245	0.646800
C	4.489670	-0.682872	1.884392
C	5.436205	-1.719501	1.890183
C	6.096594	-2.110762	0.735547
C	5.813161	-1.481907	-0.475465
C	4.850568	-0.477351	-0.545309
C	4.482824	0.159994	-1.878789
H	6.331675	-1.801275	-1.380031
H	6.833210	-2.914862	0.774297
C	3.946384	-0.264763	3.251355
H	5.659212	-2.217881	2.836900
C	0.042098	4.433615	2.781899
H	1.097578	4.573053	2.507582
H	-0.001634	4.208254	3.857939
H	-0.483564	5.385984	2.610423
H	-0.023414	2.387990	2.147080
C	-2.037740	3.041021	2.442531
H	-2.649264	3.956916	2.421508
H	-2.033892	2.672240	3.479570
H	-2.523965	2.284225	1.811122
H	2.462678	2.439141	-1.922834
C	2.154163	3.633716	-3.662244
C	1.075679	1.402102	-3.185536
H	0.705267	0.728200	-2.400225
H	1.862192	0.880324	-3.754348
H	0.241946	1.619555	-3.871991
H	2.496085	4.589878	-3.240381
H	1.394172	3.848126	-4.428475
H	3.003764	3.159762	-4.175197
C	4.668171	-0.787453	-3.066627
C	5.267088	1.454120	-2.131116
H	3.412241	0.418328	-1.825277
H	5.733439	-0.960992	-3.281546
H	4.224315	-0.344444	-3.970118
H	4.194295	-1.765327	-2.894933
H	6.347984	1.245886	-2.154717
H	5.077495	2.208422	-1.356821
H	4.981687	1.888997	-3.101348
C	2.647076	0.541629	3.339721
C	5.052535	0.480011	4.016154
H	3.763542	-1.217274	3.777141
H	5.283460	1.432483	3.513994
H	5.980572	-0.105599	4.071963
H	4.723481	0.709581	5.040396
H	2.787183	1.588835	3.034293
H	2.319153	0.549748	4.389977
H	1.837859	0.115353	2.736208
C	-1.842690	-1.262086	-0.305373
N	-3.195400	-1.310148	-0.038867
C	-1.500758	-2.425905	-1.252598
C	-0.837774	-3.632929	-0.546772
C	-0.534400	-1.983342	-2.376498
C	-2.901861	-2.793655	-1.805655
C	-3.906954	-2.441630	-0.708936
C	-5.265198	-2.036682	-1.275404

C	-4.151252	-3.639562	0.219687
H	-2.995366	-3.846242	-2.098418
H	-3.109742	-2.182941	-2.698706
H	0.186063	-3.346141	-0.295019
C	-0.785855	-4.865201	-1.465704
H	-1.320243	-3.867924	0.411244
H	0.202059	-1.292281	-1.943184
H	-1.101774	-1.403322	-3.123078
C	0.211872	-3.159077	-3.040554
C	-3.907588	-0.175304	0.484567
H	-4.663408	-4.428538	-0.349904
H	-4.797232	-3.357782	1.059800
H	-3.224644	-4.063685	0.618944
H	-5.175884	-1.255472	-2.034044
H	-5.941191	-1.684810	-0.481840
H	-5.722630	-2.916314	-1.749893
C	-4.280593	-0.075705	1.843561
C	-5.018406	1.052535	2.242886
C	-5.357354	2.066917	1.364856
C	-4.944373	1.979831	0.040162
C	-4.224331	0.878131	-0.422061
C	-3.829530	0.881896	-1.895431
H	-5.923013	2.932417	1.713424
H	-5.189145	2.784188	-0.656294
C	-3.990506	-1.045527	2.994478
H	-5.309249	1.133001	3.293264
C	-2.788300	-1.980142	2.891697
C	-5.264706	-1.804072	3.394887
H	-3.762573	-0.372844	3.838066
H	-5.617102	-2.458282	2.585443
H	-6.084337	-1.111979	3.634080
H	-5.074643	-2.430780	4.278894
H	-2.946551	-2.796797	2.181867
H	-2.606837	-2.428341	3.880142
H	-1.885463	-1.435764	2.587102
C	-2.784196	1.958570	-2.195852
C	-5.040015	1.112749	-2.815507
H	-3.381440	-0.091218	-2.134413
C	2.369856	-2.174231	-0.495372
C	1.322993	-2.183795	1.661594
C	1.833881	-3.454408	1.907723
C	2.893057	-3.444211	-0.253004
C	2.627777	-4.092524	0.951644
H	3.031356	-5.087953	1.143473
H	1.608129	-3.953550	2.852029
H	2.556585	-1.679646	-1.450132
H	3.507480	-3.929653	-1.014853
H	0.683496	-1.704298	2.405290
H	-4.768362	0.895240	-3.859374
H	-5.359088	2.164904	-2.777541
H	-5.910042	0.499129	-2.546467
H	-2.467162	1.898549	-3.249261
H	-1.896672	1.858110	-1.557395
H	-3.210644	2.959277	-2.032626
C	-0.548571	-4.480998	-2.940307
H	-1.706750	-5.463856	-1.375331
H	0.033195	-5.512007	-1.115231
H	-1.505805	-4.388811	-3.477114
H	0.009173	-5.278432	-3.452996
H	1.186240	-3.294172	-2.547042
H	0.427847	-2.916838	-4.091664

3a ν_{min} = 17 cm^{-1} *E* = -4498.1186375

C	1.825849	0.809267	0.287473
C	1.003241	-0.192256	-0.316122
C	1.636700	-1.424628	-0.859194
As	-0.819498	0.015278	0.102882
N	1.514240	2.134972	0.455743
C	2.483503	2.751249	1.231236
C	3.424278	1.823988	1.514069
N	3.031561	0.638775	0.925482
C	0.509649	2.955315	-0.184739
C	-0.419467	3.611049	0.639947
C	-1.233097	4.584732	0.049875
C	-1.153352	4.856554	-1.308788
C	0.605751	3.197142	-1.571563
C	-0.262308	4.148343	-2.112926
C	1.637048	2.490680	-2.439791
H	-0.224248	4.362525	-3.180522
H	-1.797220	5.617238	-1.752505
C	-0.584389	3.296291	2.119014
H	-1.950794	5.126147	0.669417
H	2.423504	3.808367	1.467010
H	4.346273	1.892833	2.081095
C	3.789677	-0.578962	1.080520
C	3.588816	-1.378506	2.217253
C	4.331043	-2.565317	2.292579
C	5.228690	-2.926405	1.298021
C	5.440531	-2.085573	0.207918
C	4.740700	-0.884847	0.083201
C	5.050036	0.086771	-1.048222
H	6.167092	-2.368352	-0.553439
H	5.782596	-3.862752	1.378037
C	2.724787	-1.037590	3.430040
H	4.194472	-3.213738	3.160704
C	-0.183911	4.486100	2.997982
H	0.853310	4.804098	2.820743
H	-0.283726	4.227273	4.061644
H	-0.833577	5.352063	2.801039
H	0.072451	2.448200	2.363522
C	-2.020017	2.856032	2.426422
H	-2.735183	3.675934	2.255814
H	-2.106509	2.554611	3.480808
H	-2.320147	2.002850	1.801864
H	1.654267	1.439861	-2.115152
C	3.042465	3.074972	-2.237039
C	1.278440	2.489373	-3.925194
H	0.253198	2.131871	-4.096960
H	1.967747	1.829872	-4.472017
H	1.373198	3.492238	-4.367493
H	3.388228	2.992435	-1.196256
H	3.058224	4.138971	-2.517010
H	3.767924	2.545933	-2.874044
C	5.673502	-0.578436	-2.275601
C	5.995650	1.200495	-0.570817
H	4.100264	0.555459	-1.354980
H	6.714192	-0.875302	-2.077078
H	5.697501	0.134754	-3.112046
H	5.119038	-1.469654	-2.592088
H	6.941996	0.764901	-0.217232
H	5.573216	1.800784	0.243655
H	6.224843	1.882747	-1.402559
C	1.363026	-0.384084	3.188486
C	3.541326	-0.226869	4.446605
H	2.517501	-2.011981	3.899327
H	3.760378	0.780250	4.062209
H	4.495097	-0.719888	4.678896
H	2.975390	-0.108906	5.381965
H	1.448228	0.680170	2.920292
H	0.775421	-0.430903	4.116712
H	0.790762	-0.895734	2.403114
C	-1.861486	-1.181829	-0.977933
N	-3.098137	-1.452651	-0.560747
C	-1.642759	-1.777215	-2.371006
C	-0.804316	-3.076725	-2.343877
C	-0.997801	-0.747281	-3.304057
C	-3.102071	-2.053671	-2.807775
C	-3.887755	-2.320868	-1.524081
C	-5.353476	-1.915567	-1.613784

C	-3.833067	-3.796453	-1.119460
H	-3.171588	-2.889562	-3.516426
H	-3.511656	-1.159415	-3.303103
H	0.254897	-2.866432	-2.517191
H	-1.146437	-3.749124	-3.143287
H	-0.877206	-3.611795	-1.388279
H	0.015427	-0.489964	-2.969355
H	-1.595390	0.176441	-3.343540
H	-0.931435	-1.165026	-4.320221
C	-3.720954	-0.777999	0.561781
H	-4.430030	-4.373086	-1.838930
H	-4.269692	-3.945261	-0.125381
H	-2.816953	-4.202945	-1.127318
H	-5.485908	-0.901897	-2.000488
H	-5.852395	-1.996204	-0.637144
H	-5.854140	-2.604498	-2.307629
C	-3.697242	-1.300689	1.873344
C	-4.350046	-0.556704	2.870143
C	-4.995483	0.639490	2.605917
C	-4.978519	1.149029	1.313726
C	-4.336818	0.471329	0.276869
C	-4.323884	1.154167	-1.088731
H	-5.496233	1.183201	3.407907
H	-5.461958	2.104716	1.104803
C	-3.064650	-2.593593	2.401415
H	-4.338065	-0.944040	3.891369
C	-1.866669	-3.187326	1.665263
C	-4.144649	-3.649220	2.682872
H	-2.674553	-2.297285	3.388441
H	-4.647747	-3.980681	1.764829
H	-4.919498	-3.253874	3.353599
H	-3.696974	-4.532346	3.160716
H	-2.124578	-3.599784	0.684762
H	-1.453984	-4.008571	2.268743
H	-1.075033	-2.439110	1.528267
C	-3.418402	2.390756	-1.089025
C	-5.734234	1.570944	-1.534289
H	-3.917585	0.453999	-1.830933
H	-6.077138	2.450625	-0.970714
H	-6.478656	0.777027	-1.387845
H	-5.726876	1.852116	-2.597245
H	-3.756524	3.119969	-0.336260
H	-3.451231	2.884805	-2.072131
H	-2.370672	2.144763	-0.869374
C	2.285196	-1.422606	-2.103307
C	1.594150	-2.628576	-0.136911
C	2.182627	-3.786655	-0.635403
C	2.844173	-2.592039	-2.620480
C	2.801493	-3.775830	-1.886724
H	3.246902	-4.687013	-2.288028
H	2.154004	-4.704689	-0.046365
H	2.331987	-0.500454	-2.687826
H	3.314327	-2.576849	-3.605139
H	1.108327	-2.643274	0.841004

3b ν_{min} = 16 cm^{-1} E = −4614.7129614

C	1.897778	0.993220	0.060274
C	1.034747	-0.137263	-0.065929
C	1.619932	-1.505071	-0.083961
As	-0.775339	0.267147	0.244519
N	1.625160	2.284584	-0.315793
C	2.644038	3.123160	0.109690
C	3.574718	2.353847	0.714825
N	3.127280	1.048518	0.672901
C	0.613555	2.817863	-1.201146
C	-0.250994	3.797575	-0.685657
C	-1.057333	4.491291	-1.594937
C	-1.034477	4.187013	-2.948924
C	0.647045	2.471371	-2.568424
C	-0.211812	3.166700	-3.422715
C	1.607843	1.420994	-3.105797
H	-0.219750	2.927099	-4.485678
H	-1.671238	4.736915	-3.643349
C	-0.357211	4.111915	0.798802
H	-1.724206	5.273444	-1.226673
H	2.618744	4.186684	-0.102366
H	4.523357	2.609686	1.174208
C	3.862723	-0.032660	1.280928
C	3.695588	-0.298524	2.649278
C	4.412368	-1.383616	3.172950
C	5.253020	-2.150885	2.379212
C	5.431636	-1.831018	1.035151
C	4.755456	-0.754890	0.459748
C	5.025327	-0.340230	-0.980667
H	6.112824	-2.427274	0.428551
H	5.787912	-2.997328	2.812128
C	2.893336	0.534995	3.646800
H	4.301278	-1.621784	4.233017
C	0.099673	5.541072	1.109940
H	1.133186	5.727012	0.784642
H	0.042594	5.734643	2.190489
H	-0.544007	6.275893	0.603572
H	0.295404	3.414133	1.344240
C	-1.786034	3.877141	1.301734
H	-2.494494	4.578455	0.833500
H	-1.835746	4.031573	2.389745
H	-2.123518	2.853409	1.086112
H	1.623399	0.603217	-2.370936
C	3.034477	1.974537	-3.229280
C	1.157471	0.811686	-4.433060
H	0.114040	0.467086	-4.387924
H	1.793538	-0.051136	-4.679724
H	1.249535	1.527719	-5.263244
H	3.433624	2.324107	-2.265514
H	3.057906	2.819781	-3.933385
H	3.712227	1.195440	-3.610995
C	5.569351	-1.471985	-1.852901
C	6.016230	0.833293	-1.037555
H	4.069675	-0.000601	-1.413902
H	6.612135	-1.705592	-1.590929
H	5.565489	-1.161920	-2.907781
H	4.978870	-2.390846	-1.756685
H	6.971439	0.542004	-0.575935
H	5.649148	1.728487	-0.521702
H	6.214114	1.109596	-2.083643
C	1.539974	1.094404	3.202876
C	3.774341	1.650660	4.226922
H	2.680860	-0.160121	4.474092
H	4.005629	2.406822	3.462165
H	4.722744	1.252596	4.612669
H	3.251810	2.159738	5.049645
H	1.643039	1.961505	2.532612
H	0.991600	1.443412	4.089733
H	0.920163	0.339009	2.701142
C	-1.885891	-1.227936	-0.262897
N	-3.111548	-1.240176	0.260209
C	-1.753282	-2.333942	-1.315350
C	-0.940986	-3.563797	-0.843083
C	-1.065404	-1.794850	-2.597612
C	-3.244075	-2.696640	-1.551863
C	-3.986382	-2.361843	-0.258748
C	-5.430242	-1.932799	-0.493383

C	-4.011343	-3.543248	0.714972
H	-3.394266	-3.747642	-1.824033
H	-3.644589	-2.080711	-2.372272
H	0.108523	-3.268771	-0.793984
C	-1.076134	-4.730973	-1.836209
H	-1.211959	-3.876096	0.174203
H	-0.269594	-1.092099	-2.305940
H	-1.801965	-1.206021	-3.168811
C	-0.457343	-2.909778	-3.470004
C	-3.653288	-0.153704	1.053097
H	-4.676174	-4.315251	0.304578
H	-4.413600	-3.236083	1.687390
H	-3.026598	-3.996707	0.864030
H	-5.521173	-1.168076	-1.268358
H	-5.897913	-1.567003	0.432167
H	-5.992562	-2.814010	-0.830851
C	-3.583201	-0.131083	2.463220
C	-4.168627	0.968271	3.113374
C	-4.791512	1.996740	2.427031
C	-4.817874	1.968165	1.038313
C	-4.243598	0.915794	0.325390
C	-4.270188	1.019538	-1.198017
H	-5.239580	2.828922	2.971341
H	-5.281957	2.790156	0.490885
C	-2.951961	-1.137554	3.434102
H	-4.119742	1.006014	4.203888
C	-1.823807	-2.040578	2.943189
C	-4.035176	-1.936540	4.174633
H	-2.488231	-0.489791	4.195649
H	-4.588283	-2.604884	3.501572
H	-4.768131	-1.269844	4.648678
H	-3.577762	-2.554693	4.960255
H	-2.156971	-2.795065	2.223800
H	-1.400495	-2.574695	3.806064
H	-1.017492	-1.457127	2.480871
C	-3.330522	2.119516	-1.703210
C	-5.685980	1.297325	-1.727644
H	-3.916336	0.071281	-1.625032
C	2.183138	-2.035781	-1.252557
C	1.595327	-2.310985	1.067105
C	2.112040	-3.602279	1.049867
C	2.675315	-3.342296	-1.278756
C	2.644987	-4.128488	-0.129253
H	3.035244	-5.146880	-0.149877
H	2.095295	-4.204087	1.959816
H	2.205781	-1.431838	-2.163418
H	3.080976	-3.748392	-2.207400
H	1.176818	-1.905177	1.990152
H	-5.720211	1.140046	-2.815392
H	-5.971480	2.343338	-1.544647
H	-6.448572	0.661982	-1.258183
H	-3.398549	2.200983	-2.798770
H	-2.280511	1.927907	-1.444262
H	-3.610082	3.095489	-1.276759
C	-1.176095	-4.246459	-3.295309
H	-1.941847	-5.363574	-1.585640
H	-0.189517	-5.371945	-1.717185
H	-2.229039	-4.132352	-3.597522
H	-0.749311	-4.999220	-3.972402
H	0.598961	-3.051125	-3.194055
H	-0.464472	-2.598536	-4.524252

4a ν_{min} = 17 cm^{-1} E = -4497.8266086

C	1.812563	0.790389	0.374673
C	0.929093	-0.161392	-0.324738
C	1.556362	-1.319778	-1.017004
As	-0.831660	0.178690	-0.049348
N	1.594952	2.119644	0.546010
C	2.578639	2.646024	1.346978
C	3.422192	1.628099	1.667996
N	2.953059	0.498233	1.049365
C	0.617280	2.992352	-0.081101
C	-0.367676	3.572812	0.733758
C	-1.191671	4.535361	0.139960
C	-1.054616	4.867519	-1.202535
C	0.791423	3.305825	-1.443412
C	-0.086382	4.245182	-1.989170
C	1.924156	2.715401	-2.267498
H	0.007000	4.520663	-3.039719
H	-1.706654	5.622019	-1.644846
C	-0.553357	3.213433	2.199889
H	-1.955664	5.029411	0.742938
H	2.600909	3.703365	1.593665
H	4.319428	1.608129	2.277938
C	3.656715	-0.769177	1.130039
C	3.374622	-1.645305	2.189294
C	4.063804	-2.865744	2.185221
C	4.988218	-3.175531	1.196244
C	5.282766	-2.252467	0.195112
C	4.636897	-1.015889	0.145067
C	5.055771	0.038617	-0.873115
H	6.037340	-2.496069	-0.552576
H	5.505804	-4.135468	1.218300
C	2.498593	-1.351755	3.405518
H	3.874276	-3.577756	2.991144
C	-0.121928	4.370469	3.109184
H	0.922688	4.666543	2.938743
H	-0.229198	4.088731	4.165807
H	-0.748597	5.256775	2.931442
H	0.085358	2.344107	2.424521
C	-1.997933	2.800465	2.499544
H	-2.692391	3.643659	2.364998
H	-2.085966	2.467243	3.543676
H	-2.330326	1.977928	1.849565
H	2.125739	1.704461	-1.881248
C	3.209170	3.537271	-2.090449
C	1.576909	2.564540	-3.748268
H	0.619909	2.041599	-3.891709
H	2.365868	1.996007	-4.261521
H	1.511968	3.539596	-4.251814
H	3.523734	3.592185	-1.037906
H	3.058509	4.564933	-2.451928
H	4.031642	3.089885	-2.667646
C	5.653519	-0.549715	-2.152946
C	6.090919	0.998550	-0.261643
H	4.160803	0.625097	-1.149388
H	6.664071	-0.942541	-1.969605
H	5.752406	0.238174	-2.912767
H	5.043215	-1.360710	-2.566382
H	6.984223	0.436714	0.047420
H	5.717687	1.540579	0.615268
H	6.401340	1.743661	-1.007891
C	1.164457	-0.636992	3.179483
C	3.321688	-0.632333	4.483655
H	2.248384	-2.344451	3.809909
H	3.582575	0.389313	4.168827
H	4.253366	-1.171092	4.701120
H	2.743863	-0.553878	5.415349
H	1.287885	0.438811	2.976773
H	0.559169	-0.714236	4.093873
H	0.587869	-1.089859	2.360729
C	-1.914653	-1.150317	-1.109126
N	-3.086299	-1.402601	-0.614923
C	-1.778075	-1.678675	-2.532618
C	-0.876980	-2.926854	-2.636491
C	-1.242272	-0.565223	-3.441103
C	-3.256091	-2.005123	-2.866531
C	-3.952592	-2.286545	-1.534990
C	-5.421795	-1.892723	-1.507713

C	-3.840084	-3.748963	-1.105827
H	-3.343513	-2.854817	-3.555447
H	-3.726551	-1.134381	-3.349002
H	0.174816	-2.649168	-2.740288
H	-1.164062	-3.487831	-3.536216
H	-0.963645	-3.596971	-1.771919
H	-0.199137	-0.323237	-3.195225
H	-1.850256	0.350102	-3.364718
H	-1.274725	-0.908466	-4.485549
C	-3.641054	-0.777456	0.583646
H	-4.497821	-4.340674	-1.755994
H	-4.184818	-3.881351	-0.073868
H	-2.826549	-4.150203	-1.205640
H	-5.601007	-0.884071	-1.887718
H	-5.847215	-1.985435	-0.498517
H	-5.959207	-2.591428	-2.163141
C	-3.498992	-1.336233	1.871039
C	-4.131746	-0.650850	2.922525
C	-4.863237	0.507795	2.725058
C	-4.951832	1.051807	1.448297
C	-4.339615	0.439578	0.355594
C	-4.426769	1.161062	-0.989286
H	-5.349974	0.999494	3.568051
H	-5.500298	1.982658	1.297675
C	-2.748574	-2.592488	2.326424
H	-4.036242	-1.057521	3.931497
C	-1.605397	-3.112871	1.460829
C	-3.721368	-3.716249	2.714920
H	-2.274332	-2.269424	3.267233
H	-4.277017	-4.103421	1.850785
H	-4.459044	-3.368847	3.449964
H	-3.168084	-4.554323	3.160896
H	-1.942562	-3.576654	0.527812
H	-1.054311	-3.880687	2.022427
H	-0.892687	-2.313522	1.214624
C	-3.531715	2.407026	-1.014597
C	-5.866434	1.577460	-1.328127
H	-4.070937	0.488609	-1.782708
H	-6.176553	2.442231	-0.724806
H	-6.593537	0.774332	-1.150102
H	-5.932198	1.881661	-2.382088
H	-3.812279	3.102245	-0.208592
H	-3.647782	2.936407	-1.972016
H	-2.463156	2.178743	-0.888849
C	2.166763	-1.155119	-2.268369
C	1.554629	-2.586183	-0.414548
C	2.160227	-3.667428	-1.049036
C	2.732553	-2.251946	-2.918386
C	2.740765	-3.505775	-2.307640
H	3.198444	-4.356820	-2.813496
H	2.174084	-4.642238	-0.559575
H	2.173861	-0.176529	-2.753488
H	3.174518	-2.122885	-3.907427
H	1.111217	-2.716416	0.573617

4b ν_{min} = 9 cm^{-1} E = -4614.4227557

C	1.910962	0.983294	0.117699
C	0.964912	-0.129588	-0.080972
C	1.518817	-1.501173	-0.243737
As	-0.771866	0.373692	0.051315
N	1.756822	2.262039	-0.310872
C	2.801287	3.028460	0.146022
C	3.617401	2.208252	0.861509
N	3.070741	0.951356	0.820787
C	0.785698	2.818904	-1.235790
C	-0.143844	3.746239	-0.738862
C	-0.962482	4.384248	-1.677207
C	-0.874619	4.079991	-3.030622
C	0.913063	2.491806	-2.599863
C	0.040775	3.131291	-3.483677
C	2.003024	1.562658	-3.108663
H	0.099826	2.911134	-4.549818
H	-1.522522	4.589747	-3.745074
C	-0.271662	4.084618	0.738266
H	-1.683175	5.130284	-1.337471
H	2.878348	4.083301	-0.100297
H	4.542752	2.406082	1.392649
C	3.721459	-0.192293	1.433723
C	3.447479	-0.500944	2.775088
C	4.079649	-1.640595	3.291044
C	4.945372	-2.404558	2.519078
C	5.235816	-2.029716	1.209199
C	4.642997	-0.903423	0.635734
C	5.054664	-0.433492	-0.754615
H	5.944229	-2.619806	0.628182
H	5.420311	-3.287546	2.948794
C	2.641150	0.346270	3.757237
H	3.894023	-1.917716	4.330805
C	0.236703	5.503258	1.022276
H	1.279995	5.642015	0.705439
H	0.172928	5.726047	2.096347
H	-0.371645	6.247183	0.487150
H	0.351592	3.377039	1.308171
C	-1.711249	3.915529	1.233642
H	-2.388112	4.640366	0.756194
H	-1.759298	4.087984	2.318516
H	-2.095540	2.905130	1.031423
H	2.239408	0.847800	-2.306030
C	3.284995	2.354824	-3.403694
C	1.578484	0.740853	-4.325935
H	0.627175	0.215183	-4.153424
H	2.351233	-0.005714	-4.560469
H	1.463451	1.368248	-5.221172
H	3.644970	2.898029	-2.517619
H	3.105297	3.091249	-4.200512
H	4.085510	1.678552	-3.737494
C	5.557390	-1.563363	-1.655936
C	6.160569	0.631596	-0.660466
H	4.172176	0.023955	-1.237588
H	6.560009	-1.894081	-1.348437
H	5.645546	-1.202197	-2.690211
H	4.892620	-2.434859	-1.644115
H	7.043016	0.210028	-0.157696
H	5.856133	1.526882	-0.105579
H	6.464853	0.949857	-1.667688
C	1.322684	0.954167	3.273231
C	3.538557	1.425058	4.380237
H	2.376531	-0.350087	4.567510
H	3.818303	2.187368	3.637571
H	4.460778	0.990849	4.788388
H	3.008831	1.937059	5.195921
H	1.472882	1.820219	2.609153
H	0.759717	1.322711	4.142544
H	0.692403	0.215302	2.758461
C	-1.955317	-1.225874	-0.319544
N	-3.101366	-1.174708	0.286436
C	-1.925424	-2.306428	-1.391611
C	-1.059442	-3.536637	-1.023820
C	-1.360624	-1.717064	-2.714536
C	-3.432799	-2.669639	-1.481390
C	-4.055043	-2.305271	-0.133051
C	-5.504412	-1.850086	-0.225154

C	-3.979923	-3.448482	0.879197
H	-3.599612	-3.728959	-1.707300
H	-3.910116	-2.081201	-2.279977
H	-0.013558	-3.228195	-1.061455
C	-1.275316	-4.673082	-2.038227
H	-1.241725	-3.882250	0.002560
H	-0.551836	-1.006618	-2.476366
H	-2.153347	-1.133738	-3.210169
C	-0.805109	-2.799937	-3.658502
C	-3.555053	-0.073514	1.131500
H	-4.701310	-4.217036	0.572049
H	-4.265715	-3.104207	1.879909
H	-2.992332	-3.918663	0.924638
H	-5.667736	-1.095463	-0.998150
H	-5.873555	-1.473402	0.739250
H	-6.105481	-2.729583	-0.492896
C	-3.348222	-0.046153	2.526589
C	-3.888363	1.053277	3.216197
C	-4.592846	2.060773	2.579729
C	-4.746270	2.021193	1.197962
C	-4.226393	0.972356	0.440947
C	-4.375652	1.064648	-1.077857
H	-5.007400	2.888578	3.156117
H	-5.272274	2.832079	0.692196
C	-2.609024	-1.033707	3.436677
H	-3.740840	1.104434	4.297019
C	-1.546355	-1.939368	2.822089
C	-3.587819	-1.828133	4.314815
H	-2.060937	-0.370756	4.125635
H	-4.207369	-2.518705	3.727848
H	-4.267131	-1.160553	4.860705
H	-3.031651	-2.422323	5.053051
H	-1.961215	-2.731957	2.190633
H	-0.986979	-2.430721	3.631058
H	-0.822427	-1.365897	2.226848
C	-3.440335	2.127120	-1.669369
C	-5.818824	1.385953	-1.495739
H	-4.095992	0.101433	-1.527520
C	2.025933	-1.911643	-1.483770
C	1.528831	-2.396001	0.836209
C	2.041542	-3.680422	0.678134
C	2.505268	-3.212505	-1.644485
C	2.521300	-4.095778	-0.565546
H	2.908607	-5.107494	-0.693134
H	2.062407	-4.361995	1.529623
H	2.009648	-1.229650	-2.336900
H	2.872720	-3.534391	-2.620458
H	1.162658	-2.073839	1.811764
H	-5.943932	1.220600	-2.574970
H	-6.056529	2.441691	-1.303444
H	-6.560608	0.778654	-0.960645
H	-3.605559	2.213657	-2.753560
H	-2.374752	1.903686	-1.514248
H	-3.636588	3.111666	-1.217969
C	-1.506098	-4.143084	-3.465260
H	-2.108555	-5.322532	-1.730882
H	-0.376768	-5.307486	-2.015528
H	-2.581877	-4.021811	-3.668840
H	-1.143389	-4.872248	-4.201519
H	0.270484	-2.935795	-3.463658
H	-0.893368	-2.457364	-4.698462

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