Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.


# Wanzlick's Equilibrium in Tri- and Tetraaminoolefins

# Electronic Supplementary Information (ESI)

Julian Messelberger,[‡a] Manoj Kumar,[‡a] Stephen J. Goodner[a,b], and Dominik Munz*[a,b]

*(a) Saarland University*

*Inorganic Chemistry: Coordination Chemistry*

*Campus C4.1, D-66123 Saarbrücken, Germany*

*(b) Friedrich-Alexander Universität Erlangen-Nürnberg*

*Department of Chemistry and Pharmacy: Chair of Inorganic and General*

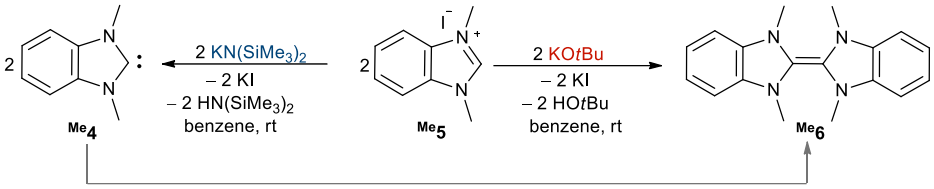
*Chemistry, Egerlandstraße 1, D-91058 Erlangen, Germany*

## Contents

# 1. General Conditions

All reactions were carried out under an atmosphere of dry dinitrogen, either in an MBraun glovebox or using standard Schlenk techniques. NMR spectra were recorded on a Bruker Avance IV 400 NMR spectrometer ($^{1}$H = 400.13 MHz, $^{13}$C = 100.60 MHz). The solvent residual signals were used as an internal reference for the $^{1}$H NMR and $^{13}$C NMR spectra. $^{1}$H NMR multiplicities are abbreviated as follows: d, doublet; dd, doublet of doublet; t, triplet; q, quartet; spt, septet; m, multiplet. All coupling constants *J* are given in Hz. Solvents were purified using a two-column solid-state purification system (MBraun; MB-SPS 5 / 7, Garching, Germany) and degassed prior to use. Pentane, Hexane, toluene, and benzene were stored over a mirror of potassium; all other solvents were stored over activated molecular sieves. Deuterated NMR solvents were obtained dry and packaged under argon and stored over activated molecular sieves or a mirror of potassium ($C_6D_6$). Benzimidazolium salt $^{Me}$**8**[1] and heterodimer salt $^{Me}$**9**[2] and olefin $^{Me}$**10**[2] were synthesized according to literature procedures. Cyclic iminium salt $^{Et}$**16** was synthesized by hydroiminiumation and subsequent salt metathesis using $NaBF_4$ in water.[3, 4] Imidazolinium salt $^{Me}$**11** was synthesized as described in the literature but using $NH_4PF_6$ instead of $NH_4BF_4$.[5]

# 2. Synthesis of $^{Me}$4 and Dimerization Kinetics




**Scheme S1**. The deprotonation of benzimidazolium salt $^{Me}$**5** by $KN(SiMe_3)_2$ and KO*t*Bu

The deprotonation of benzimidazolium salt $^{Me}$**5** (50 mg; 0.18 mmol; 1.0 eq.) by KO*t*Bu (20 mg; 0.18 mmol; 1.0 eq.) in benzene (0.6 ml) gives dimer $^{Me}$**6**. Using $KN(SiMe_3)_2$ (39 mg; 0.18 mmol; 1.0 eq.) as a base afforded predominantly the free carbene $^{Me}$**4** (56%) and the dimer $^{Me}$**6** (44%).

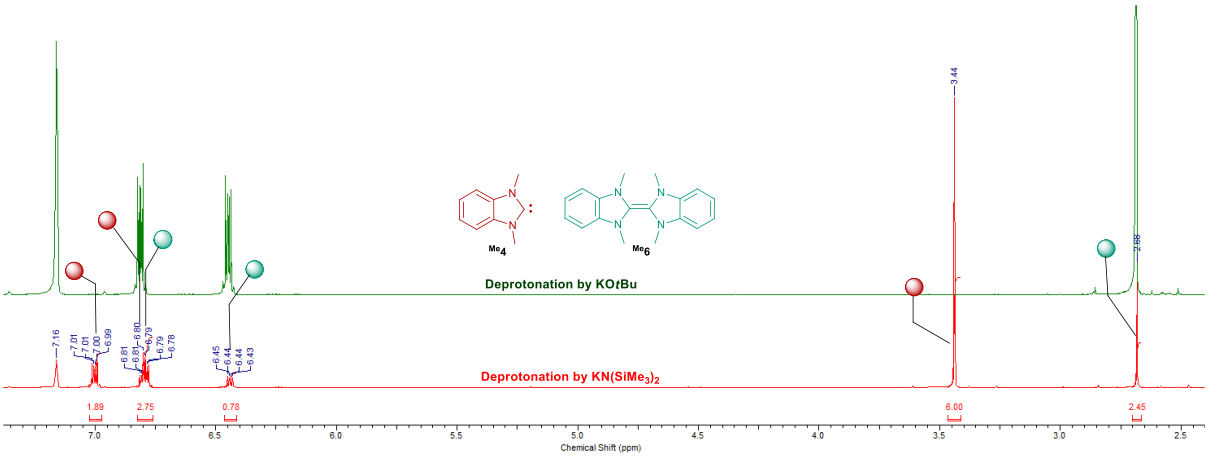



**Figure S1.** $^{1}$H NMR spectra of $^{Me}$**4** and $^{Me}$**6** (400 MHz; $C_6D_6$) after deprotonation by $KN(SiMe_3)_2$ and KO*t*Bu. Spectra were acquired approximately 5 min after the reaction.

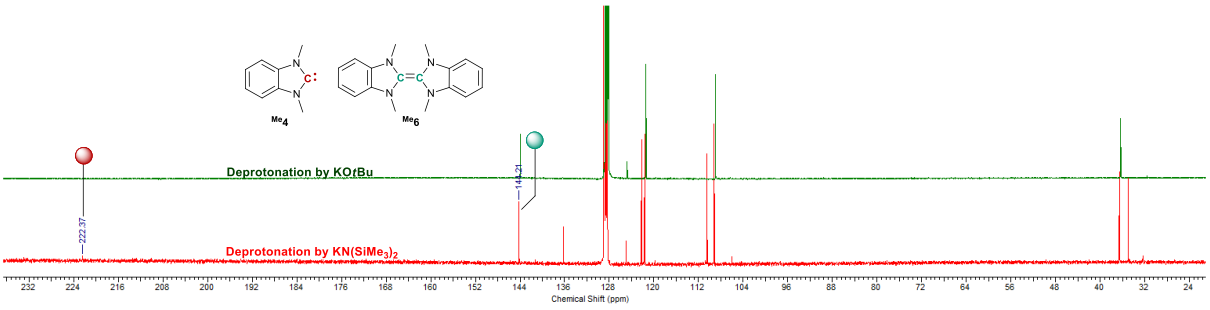
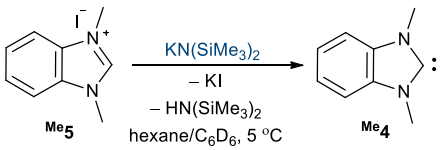



**Figure S2.** $^{13}$C NMR spectra of $^{Me}$**4** and $^{Me}$**6** (101 MHz; $C_6D_6$) after deprotonation by $KN(SiMe_3)_2$ and KO*t*Bu.



**Scheme S2**. The deprotonation of benzimidazolium salt $^{Me}$**5** by $KN(SiMe_3)_2$ at 5 °C in a mixture of benzene and hexane.

Benzimidazolium salt $^{Me}$**5** (6 mg; 0.02 mmol; 0.8 eq.), suspended in 0.5 mL of perdeutero-benzene was added slowly to a solution of $KN(SiMe_3)_2$ (11 mg; 0.05 mmol; 1.0 eq.) in 0.5 hexane at 5 °C. Quantitative deprotonation was obtained after 5 min; the *in-situ* $^1$H NMR spectroscopic analysis revealed the formation of 4% olefin $^{Me}$**6** after 1 day. Likewise, lyophilizing the mixture and redissolution in $C_6D_6$ indicated 8% dimer formation.

**$^1$H NMR** (400 MHz, $C_6D_6$) $\delta$ = 7.03 (dd, 2 H) 6.92 (dd, 2 H) 3.54 (s, 6 H) ppm; **$^{13}$C NMR** (101 MHz, $C_6D_6$) $\delta$ = 218.3 (N**C**N), 136.3 (Ar**C**N), 122.8 (Ar**C**H), 110.6 (Ar**C**H), 37.4 (N**C**H$_3$) ppm.

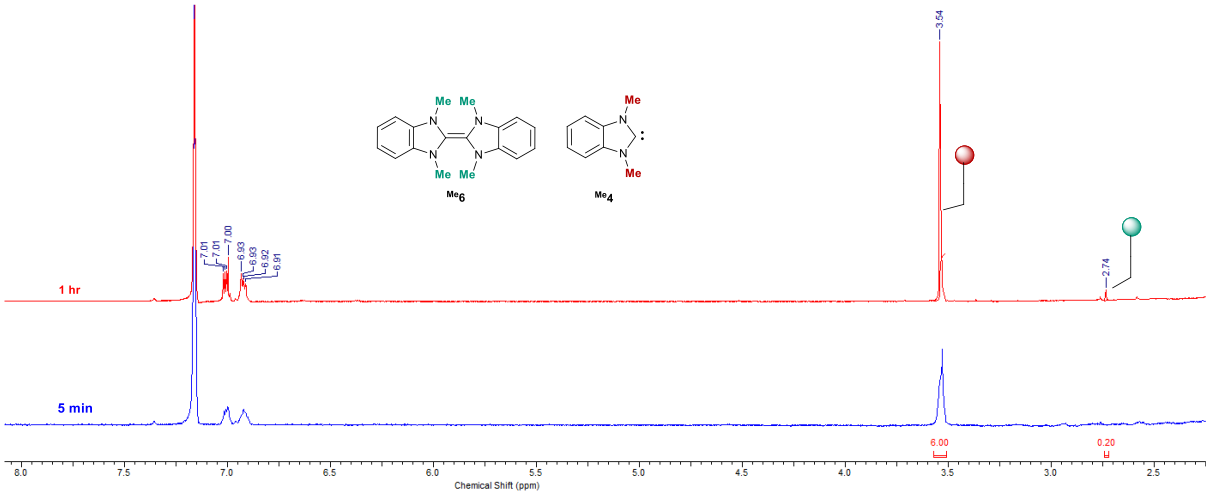



**Figure S3.** $^1$H NMR spectrum of product $^{Me}$**4** (400 MHz; $C_6D_6$ and hexane) after deprotonation by $KN(SiMe_3)_2$ at 5 °C.

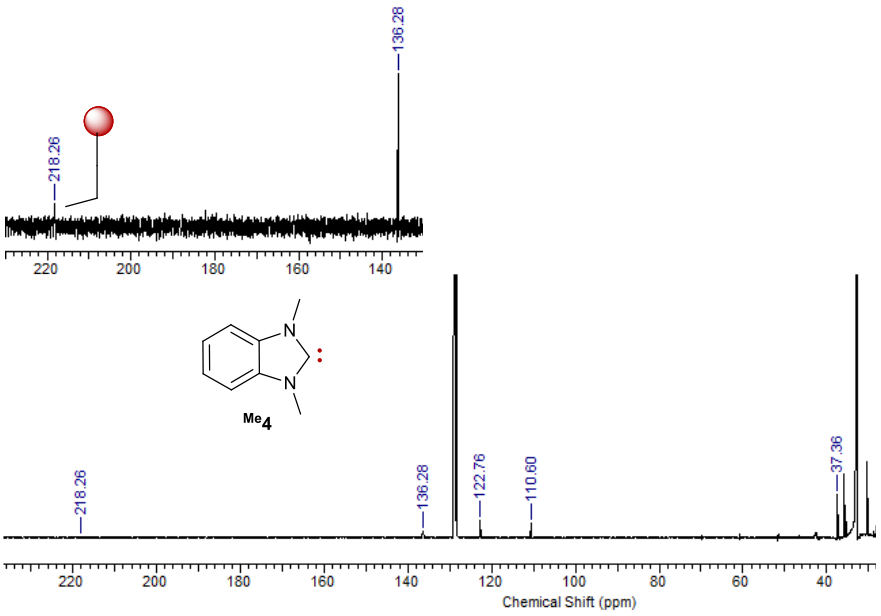



**Figure S4.** $^{13}$C NMR spectrum of product $^{Me}$**4** (101 MHz; $C_6D_6$ and hexane) after deprotonation by $KN(SiMe_3)_2$ at 5 °C.

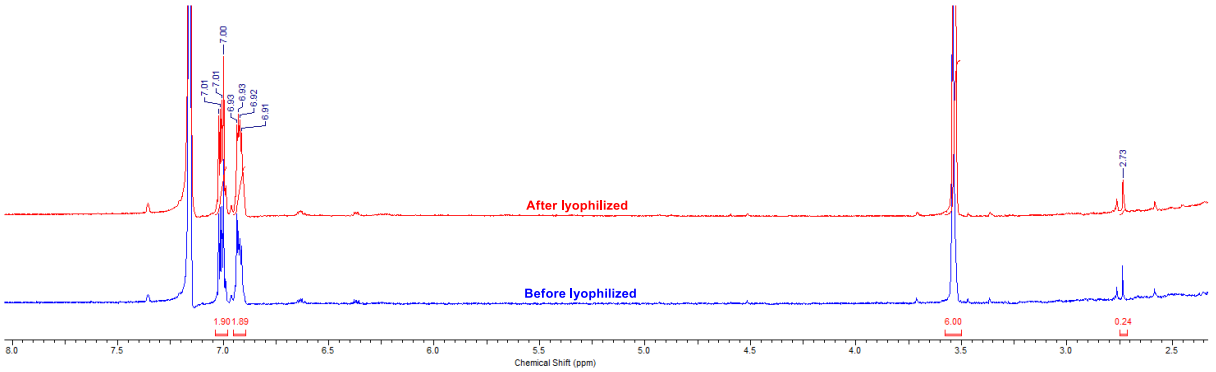
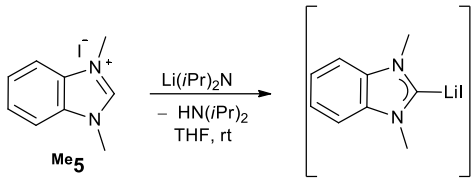



**Figure S5.** $^{1}$H NMR spectrum of product $^{Me}$**4** (400 MHz; $C_6D_6$ and hexane) and comparison to spectrum obtained in $C_6D_6$ (400 MHz; $C_6D_6$) after lyophilization.




**Scheme S3**. The deprotonation of benzimidazolium salt $^{Me}$**5** by LDA.

The benzimidazolium salt $^{Me}$**5** (50 mg; 0.18 mmol; 1.0 eq.) was added slowly to the suspension of LDA (20 mg; 0.18 mmol; 1.0 eq.) in THF (1 mL). After filtration of the reaction mixture, the lithium carbene complex with the concomitant formation of the dimer (13%) was obtained. The lithium complex converted very slowly to the homodimer $^{Me}$**6** (2% further conversion within 3 days).

**$^{1}$H NMR** (400 MHz, $C_6D_6$) $\delta$ = 6.96 (dd, 2 H) 6.73 (dd, 2 H) 3.72 (s, 6 H) ppm; **$^{13}$C NMR** (101 MHz, $C_6D_6$) $\delta$ = 207.2 (N**C**N lithium carbene), 135.4 (Ar**C**N), 122.4 (Ar**C**H), 110.5 (Ar**C**H), 50.3 (N**C**H$_3$), 34.9 (N**C**H$_3$) ppm.

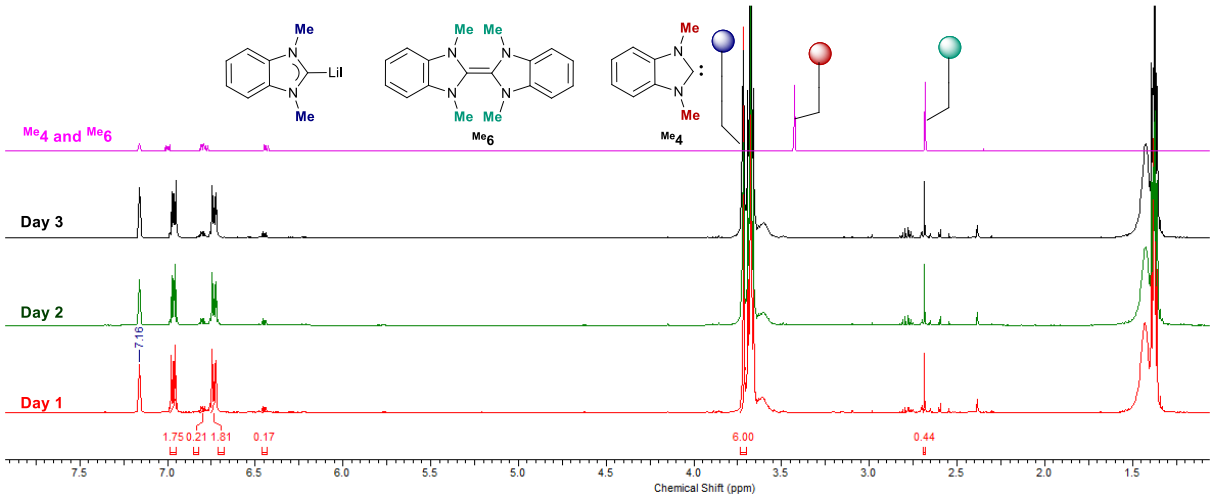



**Figure S6.** $^{1}$H NMR spectrum of the product mixture (400 MHz; $C_6D_6$) obtained after deprotonation by LDA.

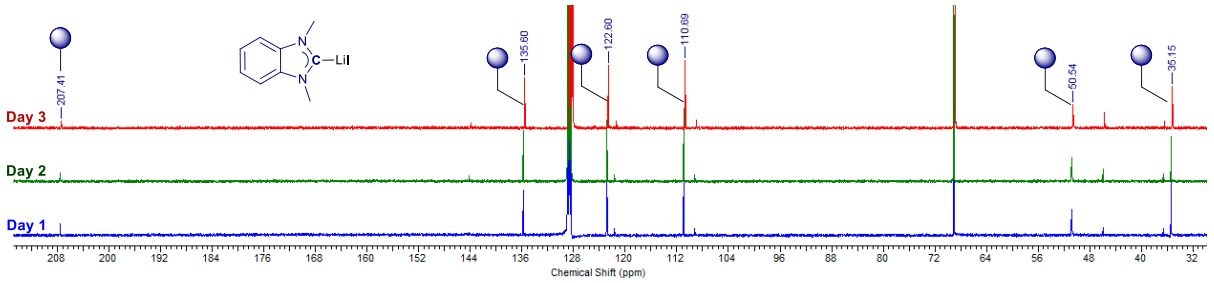



**Figure S7.** $^{13}C$ NMR spectrum of product $^{Me}$**6** and lithium complex (101 MHz; $C_6D_6$) after deprotonation by LDA.

## Kinetic Measurements

A J-Young NMR tube was charged with salt $^{Me}$**5** (50 mg, 0.18 mmol, 1.0 eq.) and $KN(SiMe_3)_2$ (39 mg, 0.18 mmol, 1.0 eq.) in $C_6D_6$ (0.6 mL) at room temperature and the composition of the resulting mixture was continuously followed by $^1H$ NMR spectroscopy.

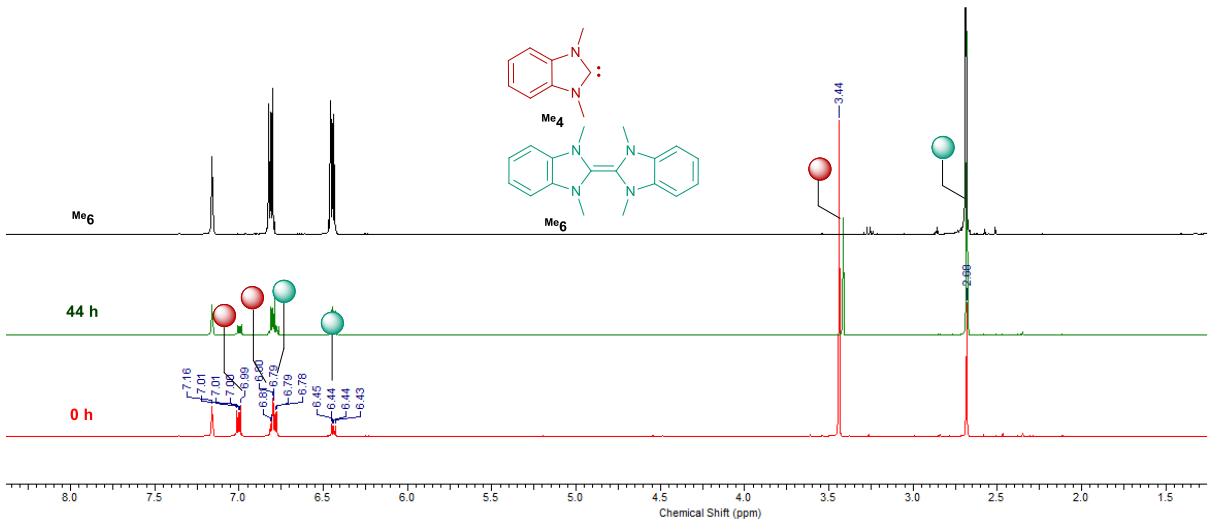



**Figure S8.** Dimerization of $^{Me}$**4** to $^{Me}$**6** according to $^1H$ NMR spectroscopy (400 MHz; $C_6D_6$).

| *Time* [h] | $c^{carbene}$ [mmol $L^{-1}$] | $c^{ln[carbene]}$ | $1/c^{carbene}$ [$mmol^{-1}$ L] | $c^{dimer}$ [mmol $L^{-1}$] | $c^{ln[dimer]}$ | $1/c^{dimer}$ [$mmol^{-1}$ L] |
|---|---|---|---|---|---|---|
| 0 | 0.71 | -0.34 | 1.40 | 0.29 | -1.26 | 3.51 |
| 1 | 0.67 | -0.40 | 1.49 | 0.33 | -1.11 | 3.04 |
| 2 | 0.64 | -0.45 | 1.57 | 0.36 | -1.01 | 2.75 |
| 3 | 0.61 | -0.49 | 1.64 | 0.39 | -0.95 | 2.58 |
| 4 | 0.59 | -0.53 | 1.69 | 0.41 | -0.89 | 2.44 |
| 5 | 0.57 | -0.56 | 1.75 | 0.43 | -0.85 | 2.34 |
| 6 | 0.55 | -0.60 | 1.80 | 0.45 | -0.81 | 2.25 |
| 7 | 0.53 | -0.64 | 1.89 | 0.47 | -0.76 | 2.13 |
| 8 | 0.51 | -0.67 | 1.94 | 0.49 | -0.72 | 2.06 |
| 9 | 0.50 | -0.69 | 1.97 | 0.49 | -0.71 | 2.03 |
| 10 | 0.49 | -0.71 | 2.01 | 0.50 | -0.69 | 2.00 |
| 11 | 0.49 | -0.73 | 2.04 | 0.51 | -0.67 | 1.96 |
| 12 | 0.47 | -0.76 | 2.10 | 0.52 | -0.65 | 1.91 |
| 13 | 0.46 | -0.78 | 2.14 | 0.53 | -0.63 | 1.88 |
| 14 | 0.45 | -0.80 | 2.20 | 0.54 | -0.61 | 1.84 |
| 15 | 0.44 | -0.82 | 2.25 | 0.56 | -0.59 | 1.80 |
| 16 | 0.44 | -0.82 | 2.27 | 0.56 | -0.58 | 1.79 |
| 17 | 0.42 | -0.85 | 2.34 | 0.57 | -0.56 | 1.75 |
| 19 | 0.41 | -0.89 | 2.42 | 0.59 | -0.53 | 1.70 |
| 21 | 0.40 | -0.92 | 2.50 | 0.60 | -0.51 | 1.67 |
| 23 | 0.38 | -0.97 | 2.59 | 0.61 | -0.49 | 1.63 |
| 25 | 0.37 | -0.98 | 2.67 | 0.63 | -0.47 | 1.60 |
| 27 | 0.35 | -1.05 | 2.79 | 0.64 | -0.44 | 1.56 |
| 29 | 0.35 | -1.05 | 2.85 | 0.65 | -0.43 | 1.54 |
| 31 | 0.34 | -1.08 | 2.91 | 0.66 | -0.42 | 1.52 |
| 33 | 0.33 | -1.11 | 2.96 | 0.66 | -0.41 | 1.51 |
| 35 | 0.32 | -1.14 | 3.09 | 0.68 | -0.39 | 1.48 |
| 37 | 0.31 | -1.15 | 3.16 | 0.68 | -0.38 | 1.46 |
| 38 | 0.31 | -1.16 | 3.18 | 0.69 | -0.38 | 1.46 |
| 40 | 0.30 | -1.20 | 3.26 | 0.69 | -0.37 | 1.44 |
| 42 | 0.29 | -1.24 | 3.40 | 0.71 | -0.35 | 1.42 |
| 44 | 0.28 | -1.27 | 3.48 | 0.71 | -0.34 | 1.40 |

**Table S1.** Evolution of concentrations of carbene $^{Me}$**5** and homodimer $^{Me}$**6**.

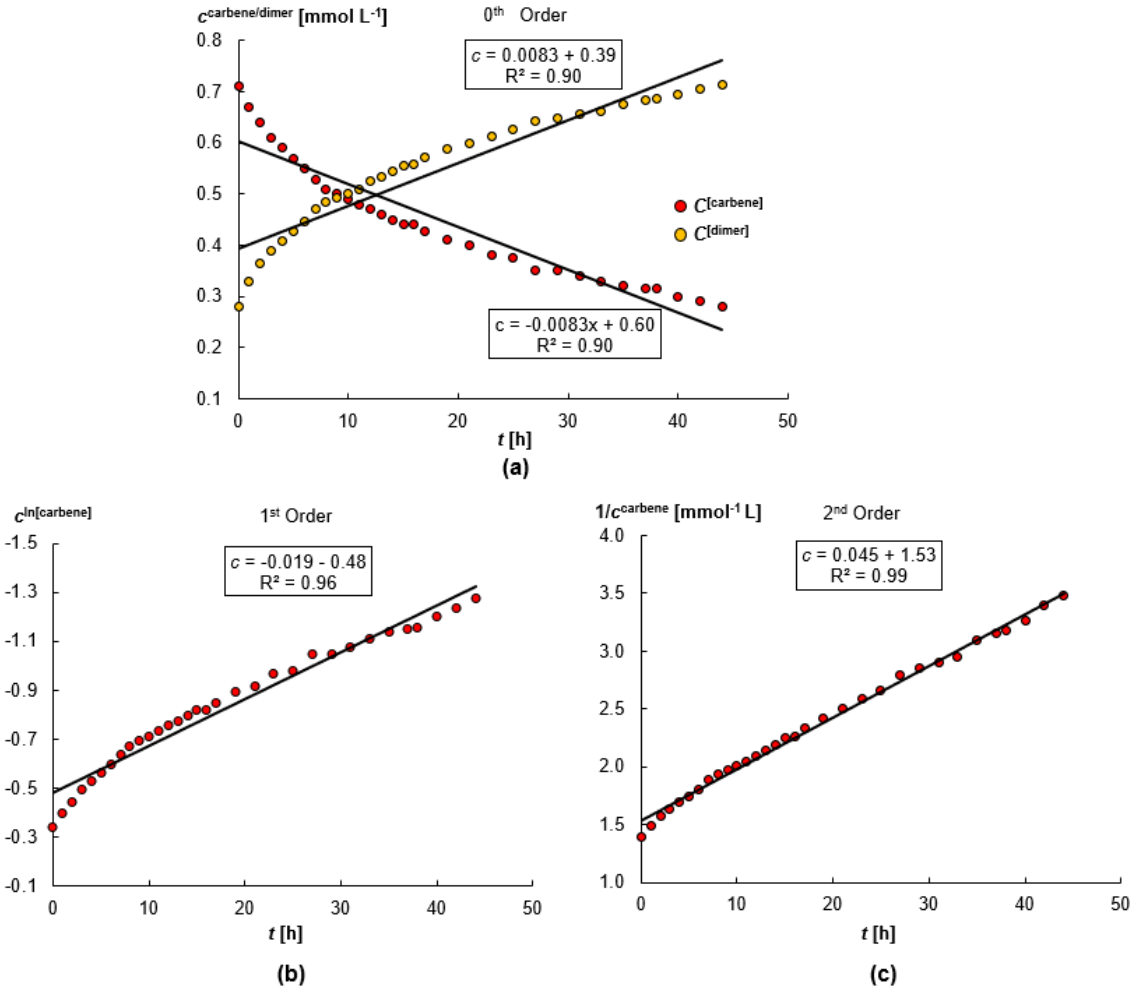
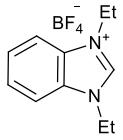



**Figure S9.** Kinetics for dimerization of carbene $^{Me}$**5** after deprotonating of benzimidazolium salt $^{Me}$**4** by KHMDS. **(a)** Zeroth order kinetic fit; **(b)** First order kinetic fit; **(c)** Second order kinetic fit.

# 3. Synthetic Procedures and Spectra

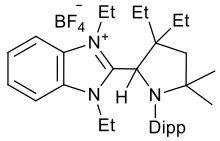
## 3.1 *N*,*N*'-Diethylbenzimidazolium Tetrafluoroborate $^{Et}$8.



$^{Et}$**8**

*N*,*N*'-Diethylbenzimidazolium tetrafluoroborate $^{Et}$**8** was synthesized according to a modified literature procedure.[6] In a pressure Schlenk tube, benzimidazole (10.2 g; 86.3 mmol; 1.0 eq.) was suspended in THF (40 mL). KO*t*Bu (9.70 g; 86.3 mmol; 1.0 eq.) in THF (20 mL) was added dropwise. The mixture was stirred for 1 h. Bromoethane (28.2 g; 19.3 mL; 259 mmol; 3.0 eq.) was added dropwise. The suspension was stirred at 100 °C for 1 h. The precipitate was filtered and washed with THF (10 mL). The colorless solid was dissolved in water (150 mL) and $NaBF_4$ (18.9 g; 173 mmol; 2.0 eq.) dissolved in water (100 mL) was added. A colorless, thick precipitate formed, was filtered off, and washed with water (200 mL) and $Et_2O$ (100 mL). Drying *in vacuo* gave the colorless product in quantitative yield (22.2 g). The analytical data corresponded to the literature data.[6]

## 2.2 CAAC–BenzNHC Salt $^{Et}$9



$^{Et}$**9**

KHMDS (223 mg; 0.11 mmol; 0.9 eq.) was added to the cyclic iminium salt $^{Et}$**14** (500 mg; 1.24 mmol; 1.0 eq.) suspended in diethyl ether (10 mL). The suspension turned immediately yellow and became a clear yellow solution over the course of 5 min. After 15 min, a fine precipitate of $KBF_4$ was observed. The reaction mixture was filtered, and volatiles were removed *in vacuo*. The yellow residue was dissolved in THF (20 mL), and 1,3-diethyl-benzimidazolium tetrafluoroborate (210 mg; 0.80 mmol; 0.8 eq.) was added. The reaction mixture was stirred overnight, during which a colorless, thick precipitate formed. The product was filtered off and washed with diethyl ether (3 × 10 mL). Drying *in vacuo* gave the colorless product in 61% yield (355 mg). **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ = 8.15 (d, *J* = 8.2 Hz, 1 H), 7.97 (d, *J* = 8.2 Hz, 1 H), 7.61 – 7.74 (m, 2 H), 7.31 (d, *J* = 7.7 Hz, 1 H), 7.21 (t, *J* = 7.6 Hz, 1 H), 6.99 (d, *J* = 7.7 Hz, 1 H), 5.16 (s, 1 H), 4.91 (m, *J* = 14.2, 6.8 Hz, 1 H), 4.55 (m, *J* = 14.9, 7.2 Hz, 1 H) ,4.27 - 4.40 (m, 1 H), 3.59 (t, *J* = 6.3 Hz, 2 H), 3.49 (sept, *J* = 13.0, 6.6 Hz, 1 H), 3.24 (sept, *J* = 13.5, 6.7 Hz, 1 H), 2.40 (dd, 2 H), 2.03 – 2.09 (m, *J* = 14.6, 7.1 Hz, 1 H), 1.81 (t, *J* = 6.9 Hz, 3 H) 1.38 (d, *J* = 6.6 Hz 3 H), 1.36 (s, 3 H), 1.32 (d, *J* = 7.4 Hz, 2 H), 1.29 (d, *J* = 6.3 Hz, 3 H), 1.25 (s, 3 H), 1.08 (d, *J* = 6.6 Hz, 3 H), 1.01

– 1.06 (m, 3 H), 0.71 (t, *J* = 7.1 Hz, 3 H), 0.56 (t, *J* = 7.0 Hz, 3 H), -0.16 (d, *J* = 6.9 Hz, 3 H) ppm; **$^{13}$C NMR** (101 MHz, DMSO-$d_6$) $\delta$ = 151.6, (N**C**N), 150.9 (Ar**C** Dipp), 149.5 (Ar**C** Dipp), 136.2 (Ar**C** Dipp), 131.4 (Ar**C** Dipp), 130.2 (Ar**C** Dipp), 128.3 (Ar**C**H), 127.5 (Ar**C**H), 127.1 (Ar**C**H), 126.2 (Ar**C**H), 124.9 (Ar**C**H), 114.8 (C**C**N), 113.8, 70.9 (**C**$_{quat}$), 67.06 (**C**H$_2$ pyrrolidine), 66.1 (**C**H$_2$ pyrrolidine), 51.1 (N**C**H$_2$ benzimidazoline), 50.3 (N**C**H$_2$ benzimidazoline), 42.9 (**C**$_{quat}$), 40.9 (**C**$_{quat}$), 31.1, 30.7 (N**C**H$_2$ pyrrolidine), 30.2 (N**C**H$_2$ pyrrolidine), 27.5, 26.9, 25.7 (CH(**C**H$_3$)$_2$ *i*Pr), 25.1 (CH(**C**H$_3$)$_2$ *i*Pr), 24.9 (CH(**C**H$_3$)$_2$ *i*Pr), 23.8 (CH(**C**H$_3$)$_2$ *i*Pr), 14.7 (NCH$_2$**C**H$_3$ benzimidazoline), 13.5 (NCH$_2$**C**H$_3$ benzimidazoline), 9.4 (CCH$_2$**C**H$_3$ pyrrolidine), 8.3 (CCH$_2$**C**H$_3$ pyrrolidine) ppm. **M.p.**: 148 – 150 ° C (decomp.) **UHR ESI–MS**: m/z calculated for $[C_{33}H_{50}N_3]^+$, $[M^+]$, 488.3999, found 488.4003.

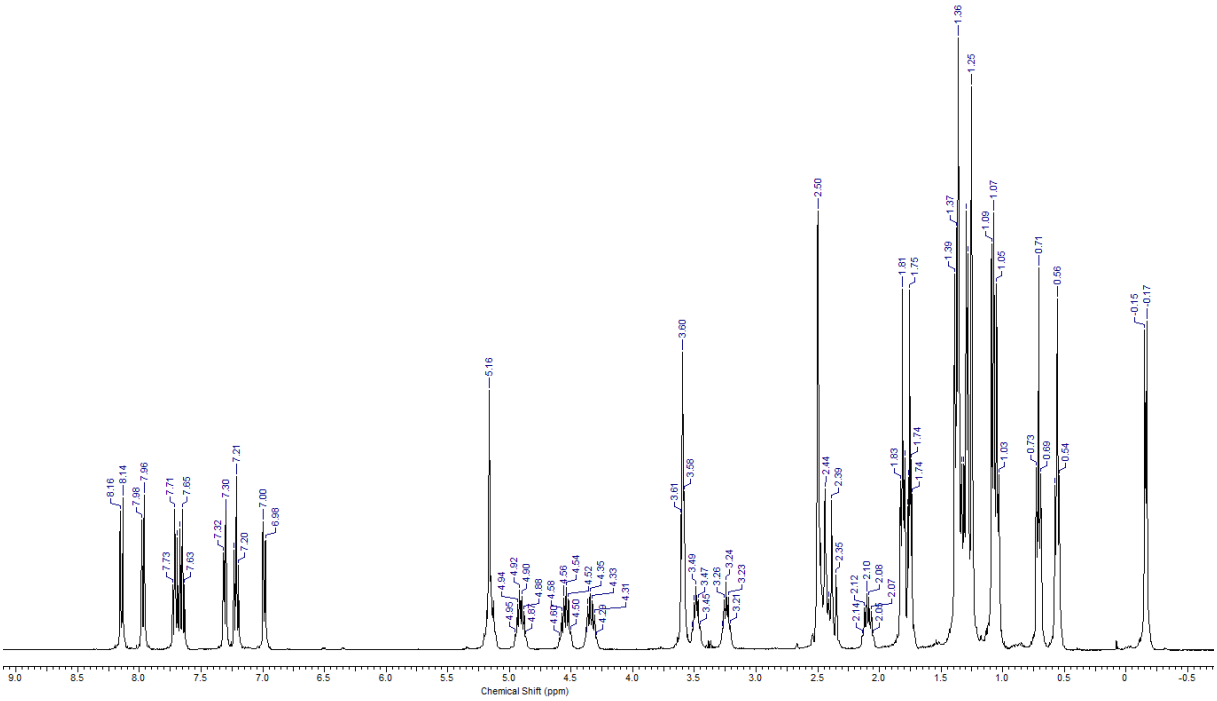



**Figure S10.** $^1$H NMR spectrum of $^{Et}$**9** (400 MHz; DMSO-$d_6$).

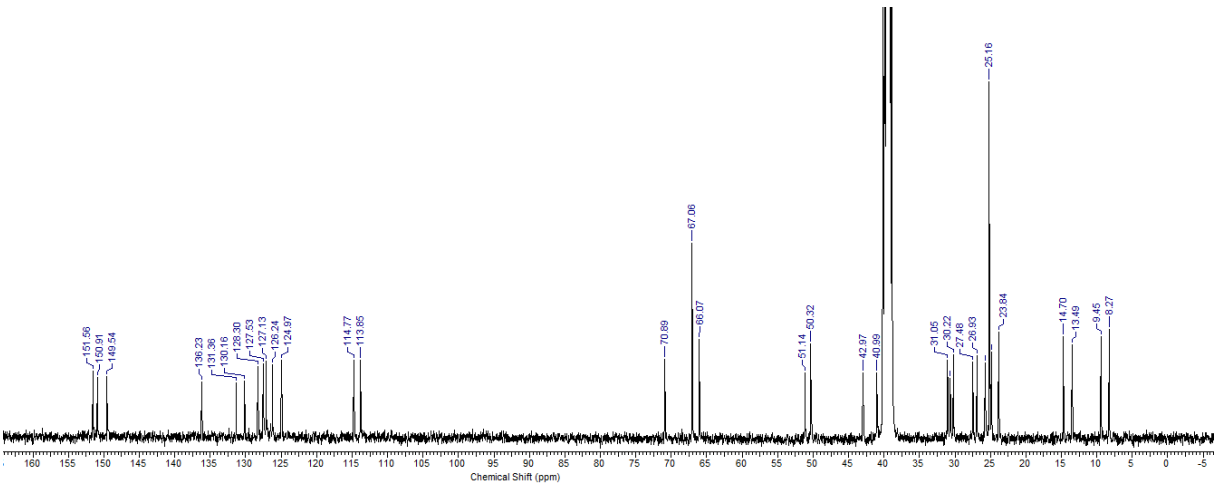
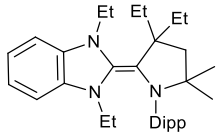



**Figure S11.** $^{13}$C NMR spectrum of $^{Et}$**9** (101 MHz; DMSO-$d_6$).

## 2.3 CAAC=BenzNHC Olefin $^{Et}$10




$^{Et}$**10**

CAAC–benzNHC salt $^{Et}$**9** (160 mg, 0.3 mmol; 1 eq.) was suspended in benzene (10 mL). KHMDS (50 mg, 0.25 mmol; 0.9 eq.) was added. After 15 min, a fine precipitate of $KBF_4$ was observed, which was filtered off. Volatiles were removed *in vacuo,* and the product was washed with hexane and drying *in vacuo* afforded the colorless solid in 80% yield (113 mg).

**$^{1}$H NMR** (400 MHz, $C_6D_6$) $\delta$ = 7.16 – 7.23 (m, 2 H), 7.14 (d, *J* = 2.4 Hz, 1 H), 7.05 (dd, *J* = 7.6, 1.0 Hz, 1 H), 6.88 – 6.93 (m, 1 H), 6.78 – 6.83 (m, 1 H), 6.68 (dd, *J* = 7.6, 0.9 Hz, 1 H), 3.47 (m, *J* = 13.4, 6.7 Hz, 2 H), 2.91 (q, *J* = 7.2 Hz, 2 H), 2.26 – 2.37 (m, 2 H), 2.06 – 2.17 (m, 2 H), 1.96 (d, *J* = 5.4 Hz, 2 H), 1.85 (s, 2 H), 1.42 (d, *J* = 6.7 Hz, 6 H), 1.29 (m, 3 H), 1.28 (s, 3 H), 1.25 – 1.28 (m, 6 H), 1.12 (s, 6 H), 1.04 (t, *J* = 7.5 Hz, 6 H), 0.61 (t, *J* = 7.1 Hz, 3 H) ppm; **$^{13}$C NMR** (101 MHz, $C_6D_6$) $\delta$ = 150.1 (N**C**N), 147.4 (Ar**C** Dipp), 145.6 (Ar**C** Dipp), 143.8 (Ar**C** Dipp), 141.1 (Ar**C** Dipp), 127.6 (Ar**C**N), 124.9 (Ar**C**H), 123.3 (Ar**C**H), 116.0 (Ar**C**H), 114.3 (C**C**N), 63.4 (**C**$_{quat}$), 54.9 (N**C**$H_2$ benzimidazoline), 50.6 (**C**$_{quat}$), 46.8 (NC**C**$H_2$ pyrrolidine), 46.5 ($CCH_2$**C**$H_3$ pyrrolidine), 32.5 (**C**H$(CH_3)_2$ *i*Pr), 30.1 (**C**H$(CH_3)_2$ *i*Pr), 28.7 (NC**C**$H_3$ pyrrolidine), 25.8 (CH(**C**$H_3)_2$ *i*Pr), 25.1 (CH(**C**$H_3)_2$ *i*Pr), 15.6 ($NCH_2$**C**$H_3$ benzimidazoline), 13.3 ($NCH_2$**C**$H_3$ benzimidazoline) 10.7 ppm. **M.p.**: 161 – 163 °C; **UHR ESI–MS**: m/z calculated for $[C_{33}H_{49}N_3]^+$, $[M^+]$ 487.3921, found 487.3906.

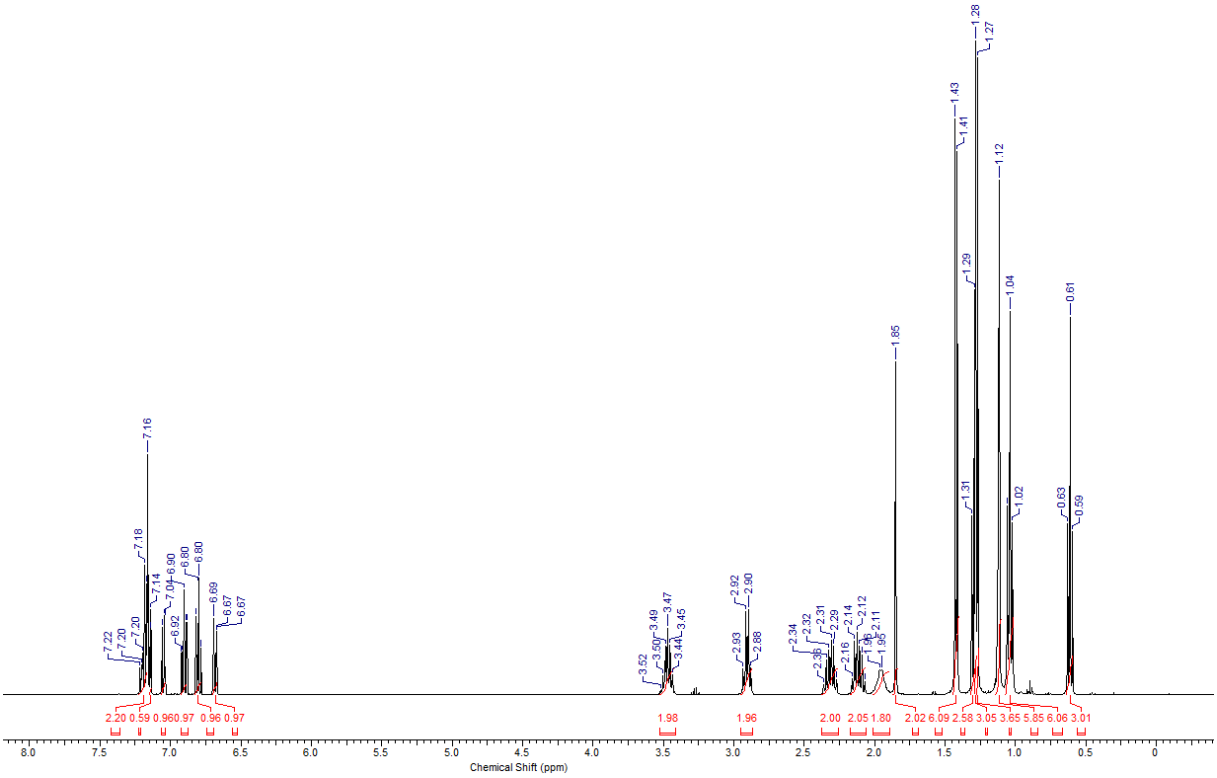



**Figure S12.** $^{1}$H NMR spectrum of $^{Et}$**10** (400 MHz; $C_6D_6$).

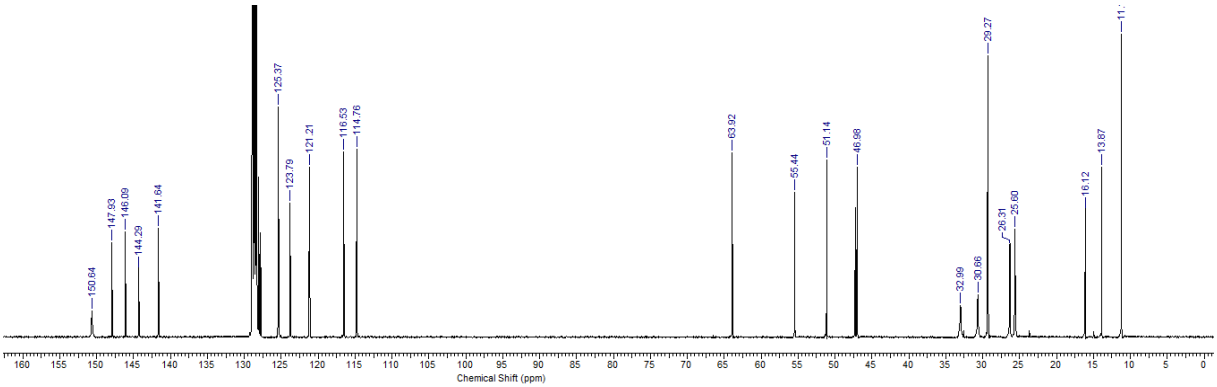
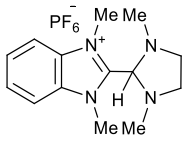



**Figure S13.** $^{13}$C NMR spectrum of $^{Et}$**10** (101 MHz; $C_6D_6$).

## 2.4 saNHC–BenzNHC Salt $^{Me}$12




$^{Me}$**12**

1,3-Dimethyl-benzimidazolium iodide $^{Me}$**5** (500 mg; 0.18 mmol; 1.0 eq.) was suspended in diethyl ether (7 mL). KHMDS (328 mg; 0.16 mmol; 0.9 eq.) was added. The suspension turned immediately yellow. After 15 min, a fine precipitate of KI was observed, which was filtered off. All volatiles were removed *in vacuo*, and the residue was dissolved in THF (20 mL). 1,3-dimethyl-imidazolinium hexafluorophosphate (445 mg; 0.18 mmol; 0.9 eq) was added, and the reaction was stirred for 1 h. The product was filtered off and washed with diethyl ether (15 ml). Drying in vacuo gave the colorless product in 65% yield (509 mg) as a mixture with $^{Me}$**8** (15%) and $^{Me}$**11** (5%). Repeated crystallization, as well as redissolution in various solvents (DMSO-$d_6$, CDCl3, $CD_3CN$, pyridine-$d_5$) always indicated the presence of the imidazolinium ($^{Me}$**11**)/benzimidazolium salts ($^{Me}$**8**). The same was observed *in-situ* when performing the reaction in DMSO-$d_6$ (Fig. S14). **$^1$H NMR** (400 MHz, DMSO-$d_6$) $\delta$ = 8.06 (dd, $J$ = 6.2, 3.1 Hz, 2 H), 7.72 (dd, $J$ = 4, $J$=3 Hz, 2 H), 4.62 (s, 1 H), 4.19 (s, 6H), 3.37 – 3.42 (m, 2 H), 2.72 – 2.78 (m, 2 H), 2.36 (s, 6 H) ppm; **$^{13}$C NMR** (101 MHz, DMSO-$d_6$) $\delta$ = 148.9 (N**C**N benzimidazoline), 132.1 (Ar**C**N), 126.7 (Ar**C**H), 113.4 (N**C**N imidazolidine), 81.1, 53.6 (**C**$H_2$ imidazolidine backbone), 33.7 (N**C**$H_3$ imidazolidine), 32.2 (N**C**$H_3$ benzimidazoline) ppm. **M.p.**: 190 – 195 °C (mixture; decomp.).

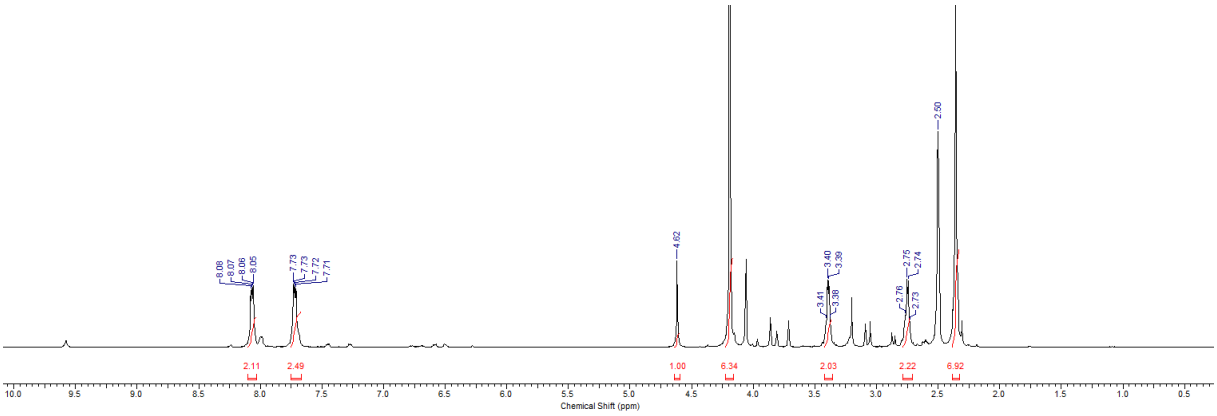



**Figure S14.** $^{1}$H NMR spectrum of $^{Me}$**12** (400 MHz; DMSO-$d_6$).

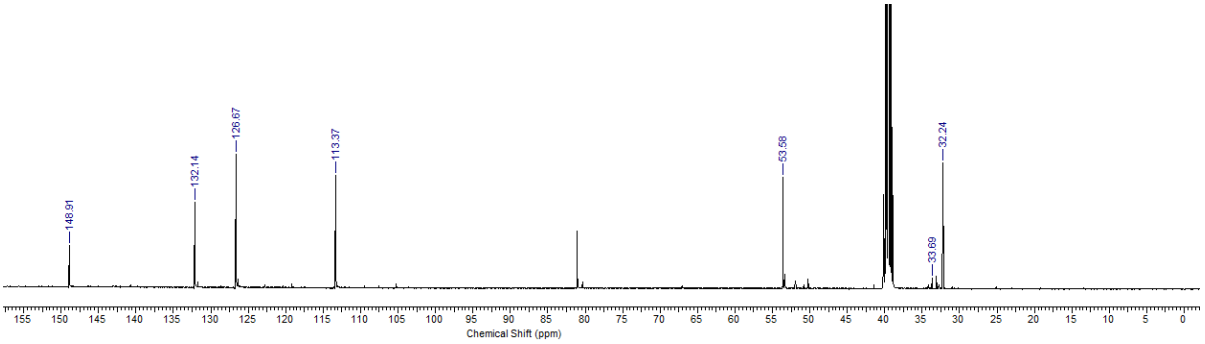
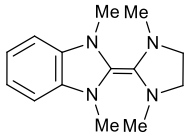



**Figure S15.** $^{13}$C NMR spectrum of $^{Me}$**12** (101 MHz; DMSO-$d_6$).

## 2.5 saNHC=BenzNHC Olefin $^{Me}$13




$^{Me}$**13**

saNHC–BenzNHC salt $^{Me}$**12** (100 mg; 0.25 mmol; 1.0 eq.) was suspended in benzene (10 mL) and KHMDS (41 mg; 0.2 mmol; 0.8 eq.) was added. After 15 min, a fine precipitate of $KPF_6$ was observed, which was filtered off. Drying *in vacuo* gave a yellow, viscous oil, which was triturated with hexane. A fine yellow powder was obtained after lyophilization with benzene in 92% yield (68 mg). **$^{1}$H NMR** (400 MHz, $C_6D_6$) $\delta$ = 6.81 (dd, $J$ = 5.5, 3.1 Hz, 2 H) 6.41 (dd, $J$ = 5.5, 3.1 2 H) 3.09 (s, 6 H) 2.63 (s, 4 H) 2.30 (s, 6 H) ppm; $^{13}$C NMR (101 MHz, $C_6D_6$) $\delta$ = 141.9 (N**C**N benzimidazoline), 129.9 (Ar**C**N), 123.1 (Ar**C**H benzimidazoline), 120.0 (Ar**C**H benzimidazoline), 106.1 (N**C**N imidazolidine), 51.5 (**C**$H_2$ imidazolidine backbone), 41.9 (N**C**$H_3$ imidazolidine), 33.3 (N**C**$H_3$ benzimidazoline) ppm. **M.p.**: 42 – 44 °C; **UHR ESI–MS**: m/z calculated for $C_{14}H_{21}N_4^+$, $[M+H]^+$ 245.1760, found. 245.1759.

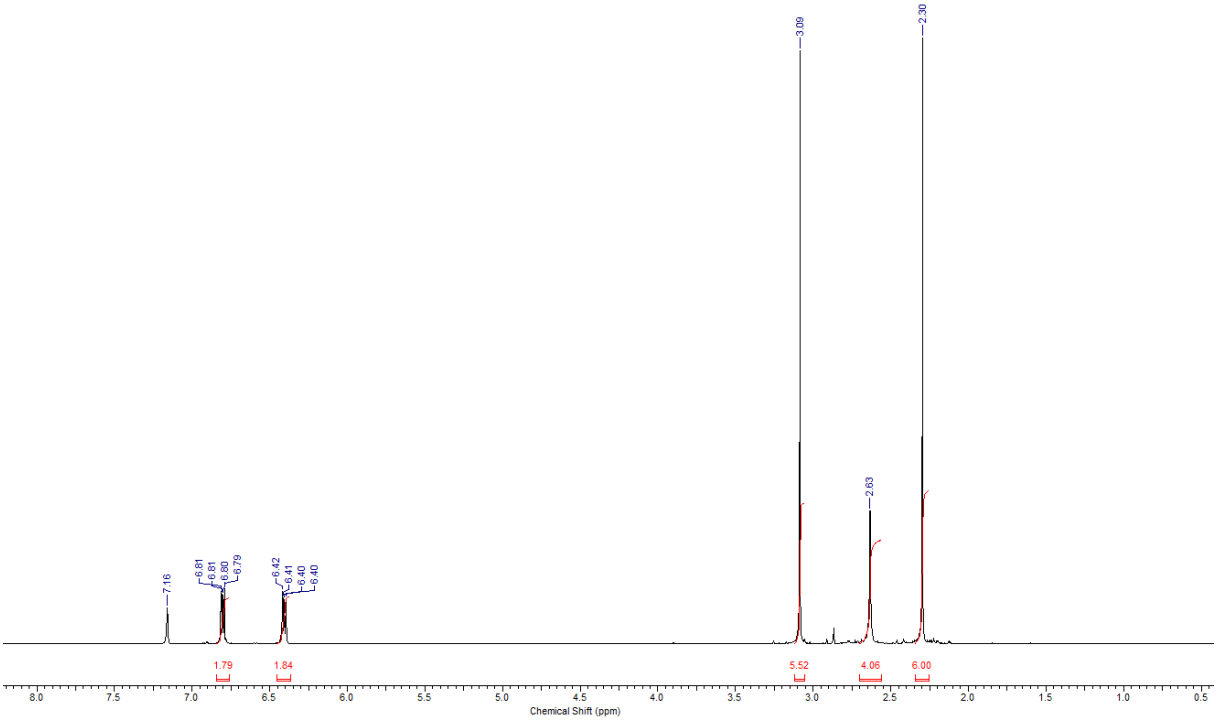



**Figure S16.** $^{1}$H NMR spectrum of $^{Me}$**13** (400 MHz; $C_6D_6$).

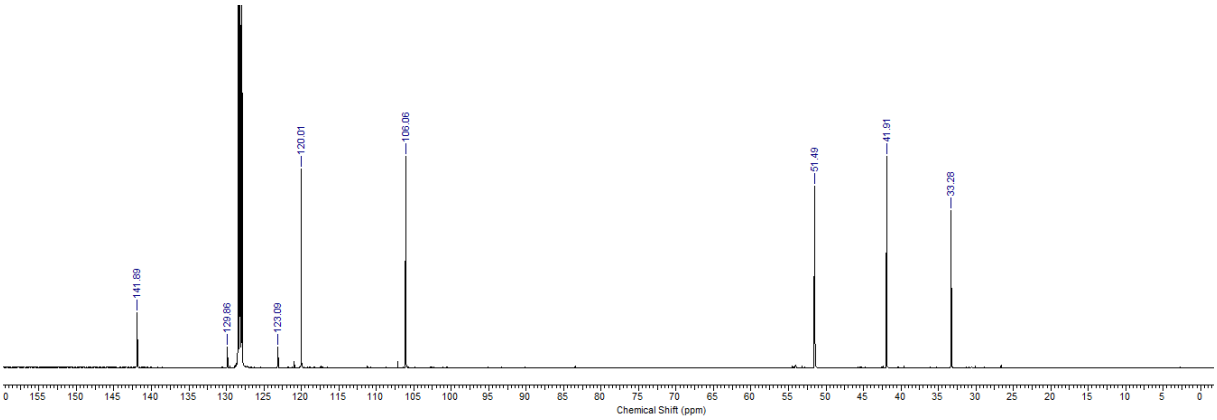
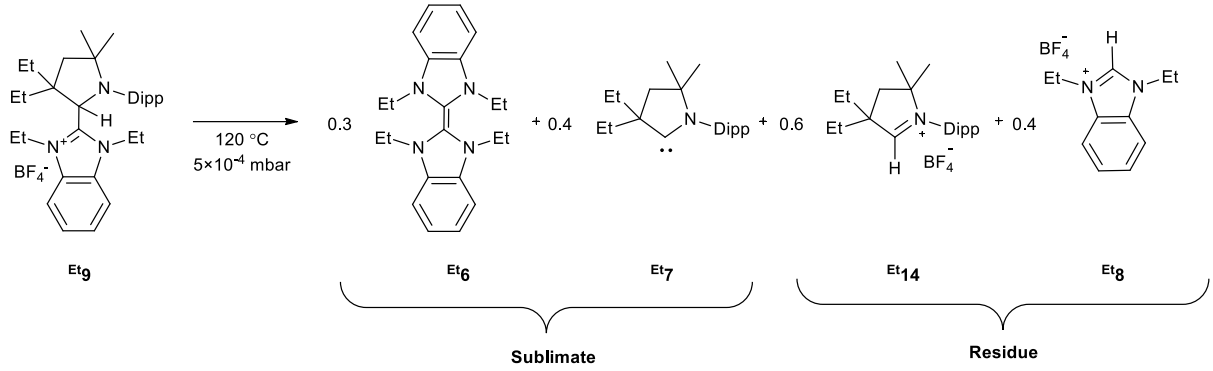



**Figure S17.** $^{13}$C NMR spectrum of $^{Me}$**13** (101 MHz; $C_6D_6$).

# 4. Sublimation Experiments

## 4.1 Sublimation of CAAC–BenzNHC Salt $^{Et}$9




Dissociation of the adduct $^{Et}$**9** (50 mg) was performed in a sublimation flask under heating in an oil bath. The protonated cyclic iminium salt and 1,3-diethyl-benzimidazolium tetrafluoroborate were obtained in the residue, which was off-white to slightly brownish. The homodimer $^{Et}$**10** crystallized on the sides of the flask wall as a yellow, crystalline material, whereas $^{Et}$**7** formed a faint yellow, greasy solid.

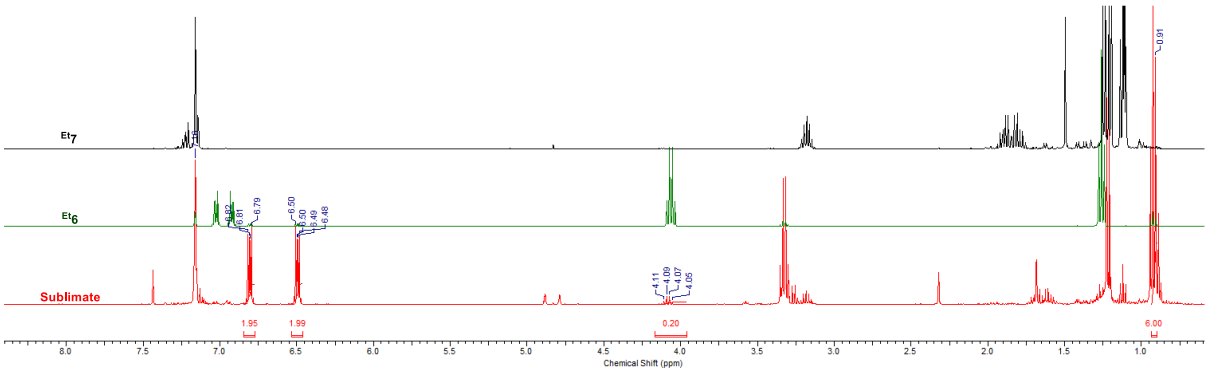



**Figure S18.** Stacked $^{1}$H NMR spectra of sublimed products, $^{Et}$**6** and $^{Et}$**7** (400 MHz; $C_6D_6$).

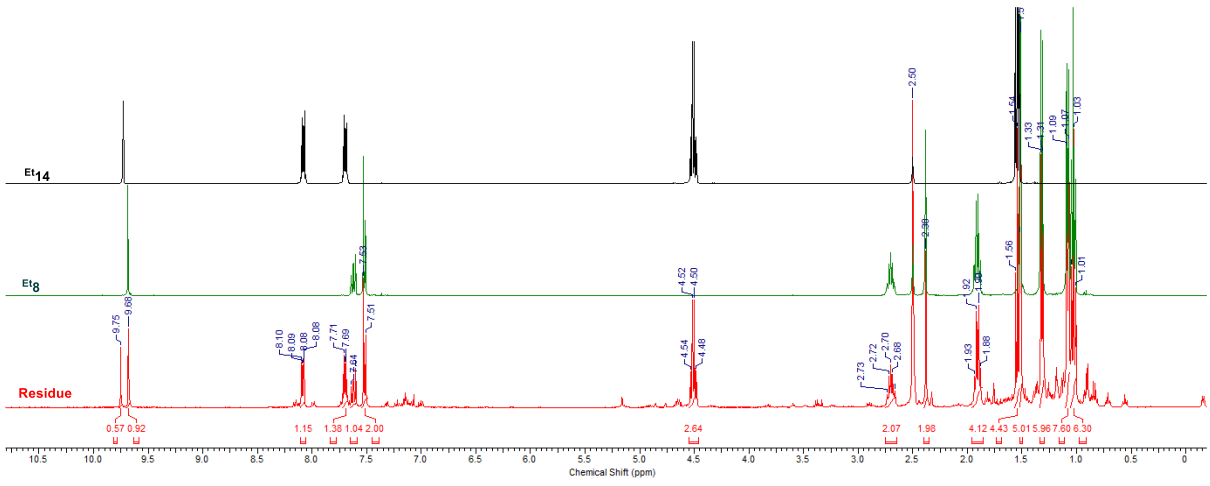
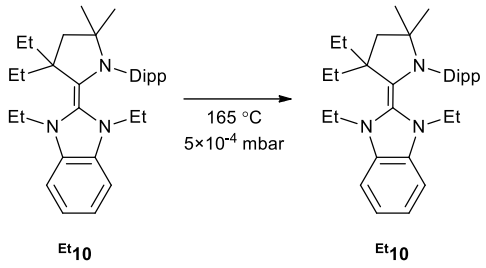



**Figure S19.** Stacked $^{1}$H NMR spectra of residue indicating the concomitant presence of $^{Et}$**14** and $^{Et}$**8** (400 MHz; DMSO-$d_6$).

## 4.2 Sublimation of CAAC=BenzNHC Olefin $^{Et}$10




$^{Et}$10 $^{Et}$10

Dissociation of the adduct $^{Et}$**10** (50 mg) was performed in a sublimation flask under heating in an oil bath. The homodimer $^{Et}$**10** formed as a yellow crystalline material at the flask walls.

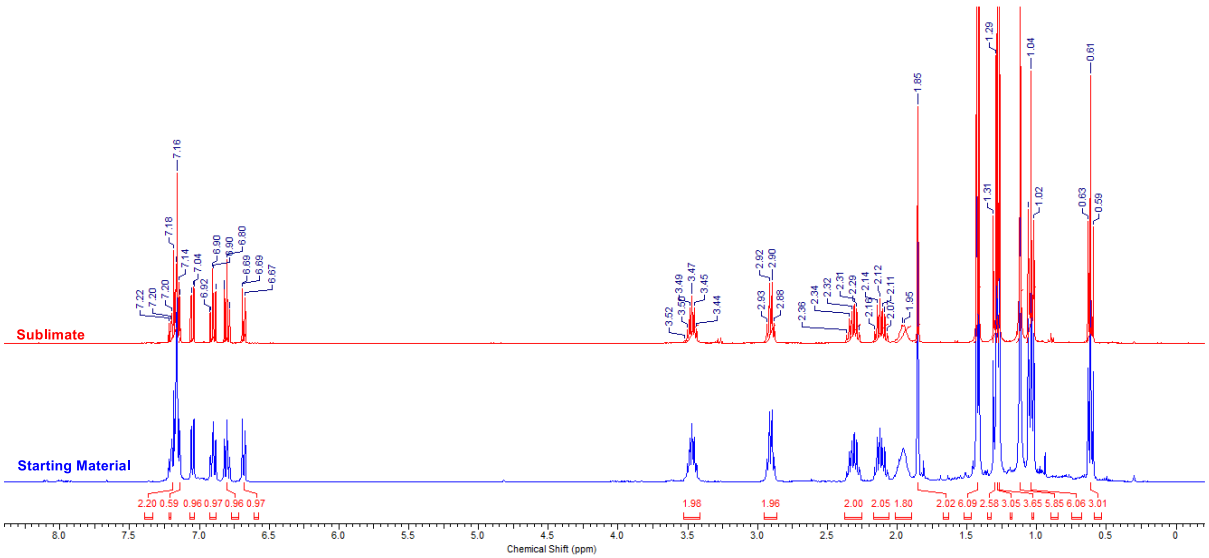
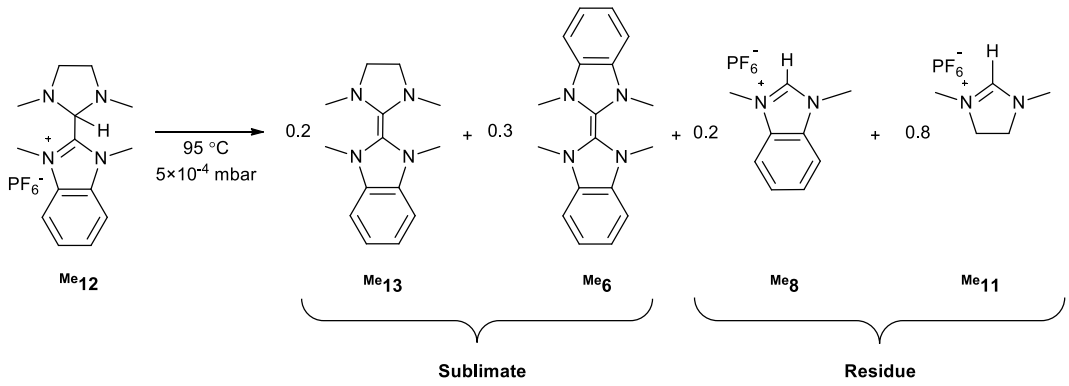



**Figure S20.** Stacked $^{1}$H NMR spectra of $^{Et}$**10** before (blue) and after (red) sublimation (400 MHz; $C_6D_6$).

## 4.3 Sublimation of saNHC–BenzNHC Salt $^{Me}$12




$^{Me}$12 $^{Me}$13 $^{Me}$6 $^{Me}$8 $^{Me}$11

Sublimate Residue

Dissociation of the saNHC-benzNHC $^{Me}$**12** (50 mg) was performed in a sublimation flask under heating in an oil bath. The heterodimer $^{Me}$**13** and homodimer $^{Me}$**6** were obtained as a yellow crystalline material at the flask walls. In addition, the protonated benzNHC salt $^{Me}$**8** and saNHC salt $^{Me}$**11** were obtained in the colorless residue.

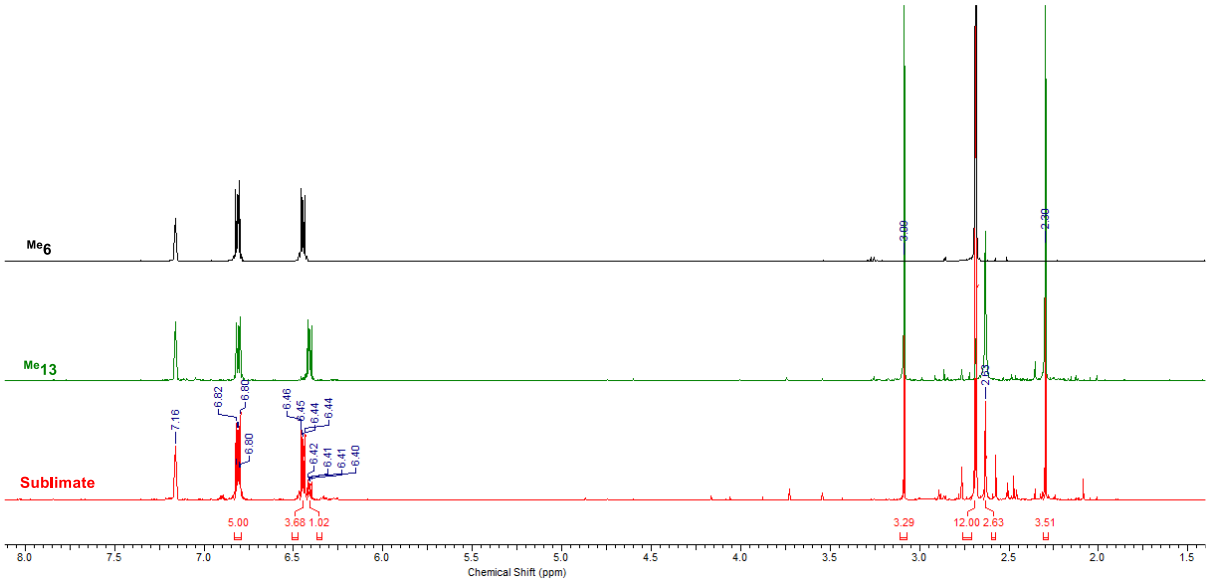



**Figure S21.** Stacked $^{1}$H NMR spectra of the sublimed products with hetero $^{Me}$**13** and homodimer $^{Me}$**6** (400 MHz; $C_6D_6$).

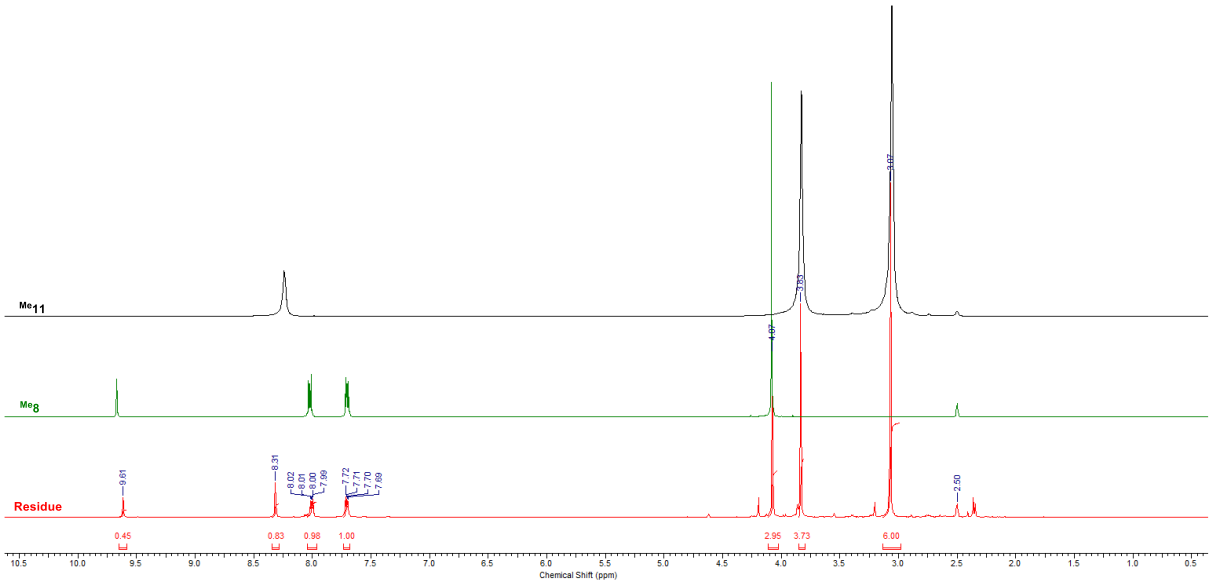
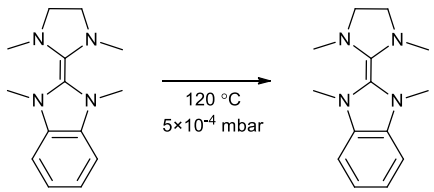



**Figure S22.** Stacked $^{1}$H NMR spectra of residue, benzNHC $^{Me}$**8,** and saNHC salt $^{Me}$**11** (400 MHz; DMSO-$d_6$).

## 4.4 Sublimation of saNHC=BenzNHC Olefin $^{Me}$13




$^{Me}$**13** $^{Me}$**13**

Dissociation of the olefin $^{Me}$**13** (50 mg) was performed in a sublimation flask under heating in an oil bath. The homodimer $^{Me}$**13** formed as a yellow crystalline material at the flask walls.

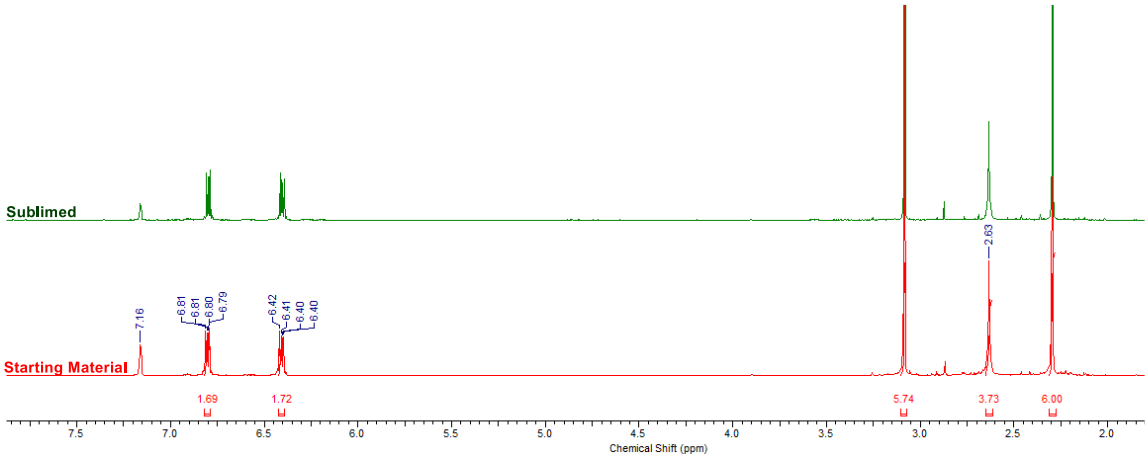
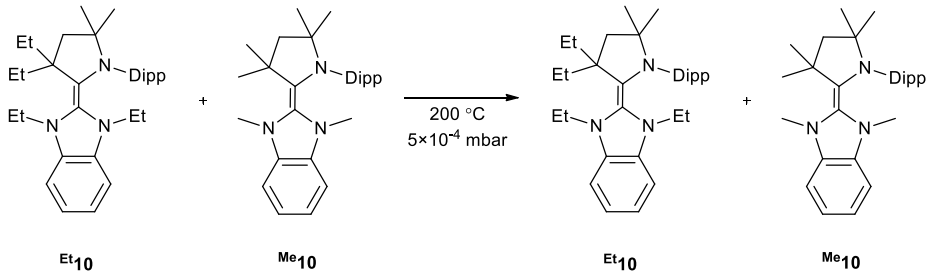



**Figure S23.** Stacked $^{1}$H NMR spectra of $^{Me}$**13** before (red) and after (green) sublimation (400 MHz; $C_6D_6$).

## 4.5 Sublimation Crossover Experiment




$^{Et}$**10** $^{Me}$**10** $^{Et}$**10** $^{Me}$**10**

Olefins $^{Et}$**10** and $^{Me}$**10** were ground and put mixed in the sublimation flask. Upon slowly elevating the temperature to 185 °C, only the methyl olefin $^{Me}$**10** sublimed, leaving $^{Et}$**10** in the residue. However, when the temperature was adjusted rapidly to 200 °C, crystallization along the flask wall was an equal mixture of both dimers, with no crossover products, thus disproving dissociation.

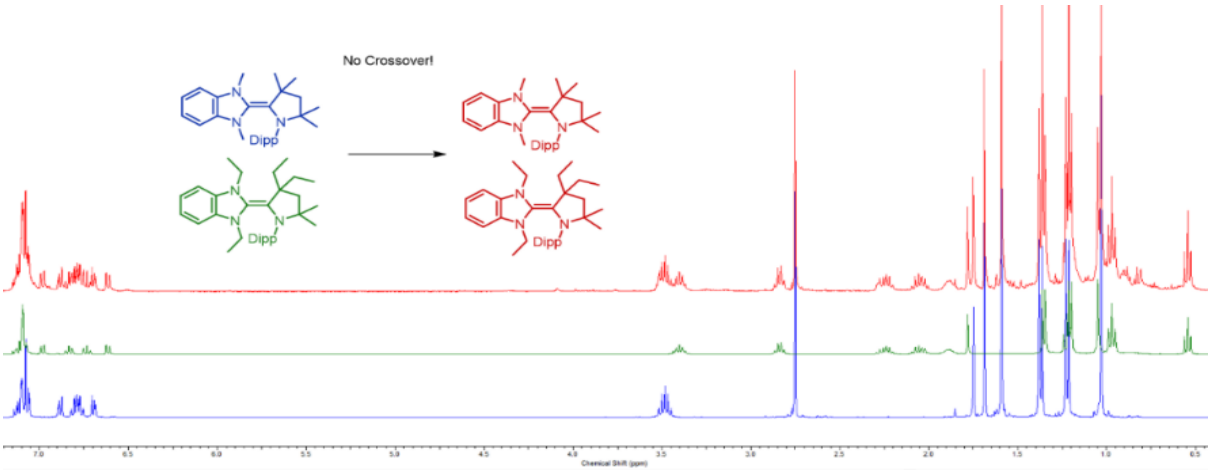



**Figure S24.** Stacked $^{1}$H NMR spectra of starting material ($^{Me}$**10** and $^{Et}$**10**) and sublimation of a mixture of the two products (400 MHz; $C_6D_6$).

# 5. Computational Details

The calculations were performed with ORCA v. 4.2.1.[7, 8] All geometric parameters were optimized without constraints at the BLYP-D3BJ/def2-TZVPP level of theory.[9-14] This method was chosen according to previous computational studies,[15, 16] a benchmark with B3LYP[17, 18] and PBEh-3c[19] which revealed an inferior fit with the experimental results, and in sight of difficulties to localize transition states at the double-ζ level of theory (note the very low imaginary frequencies given below). The RI approximation and the related auxiliary basis set (def2/J)[20] were used to speed up the calculations. Tighter than default convergence criteria were chosen for both the optimization (*tightopt*) of the structural parameters as well as the scf (*tightscf*), and more accurate than default grid values (*Grid6*, *FinalGrid7*) were used. All calculated structures were verified as true minima by the absence ($N^{\text{imag}} = 0$) of negative eigenvalues in the harmonic vibrational frequency analysis, or as first-order transition states ($N^{\text{imag}} = 1$), respectively. The energies of all structures were corrected by single-point calculations at the DLPNO-CCSD(T)[21, 22]/def2-TZVPP[13, 14] level of theory using the def2-TZVPP/C auxiliary basis set[14] and "*NormalPNO*" settings.[23] Implicit correction for solvation effects (solvent: THF) was conducted with the Conductor-like Continuum Polarization (CPCM) model using point charges according to the Gaussian Charge Scheme with van-der-Waals surface cavities.[24]

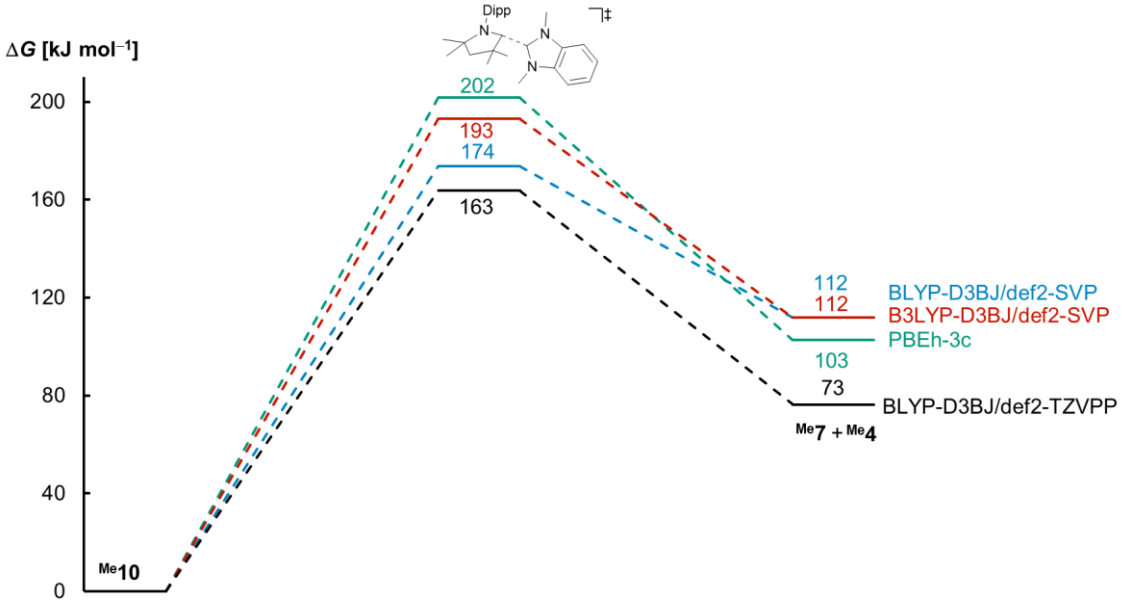



**Figure S25**. Comparison of functionals.

## Energies

| | $N^{imag}$ | $\Delta E$ | $\Delta G$ | $\Delta E$ | $\Delta E$ (GCS=THF) |
|---|---|---|---|---|---|
| **Basis set** | | **def2-TZVPP** | **def2-TZVPP** | **def2-TZVPP** | **def2-TZVPP** |
| **Method** | | **BLYP-D3** | **BLYP-D3** | **DLPNO-CCSD(T)//BLYP-D3** | **BLYP-D3//BLYP-D3** |
| $^{Me}$**4** | 0 | -458.4781009 | -458.3438655 | -457.6247942 | -458.4881573 |
| $^{Et}$**4** | 0 | -537.0995923 | -536.9128481 | -536.1108755 | -537.1097636 |
| $^{Me}$**7** | 0 | -835.4776168 | -835.0724658 | -833.9774893 | -835.4876832 |
| $^{Et}$**7** | 0 | -914.0917649 | -913.6337859 | -912.4564569 | -914.1012394 |
| $^{Me}$**9** | 0 | -1294.460948 | -1293.87617 | -1292.114774 | -1294.521121 |
| **TS** $^{Me}$**9** | 1 (–23 $cm^{-1}$) | -1294.427083 | -1293.848062 | -1292.069872 | -1294.48595 |
| $^{Et}$**9** | 0 | -1451.698902 | -1451.006769 | -1449.080462 | -1451.756602 |
| **TS** $^{Et}$**9** | 1 (–21 $cm^{-1}$) | -1451.664576 | -1450.980058 | -1449.035539 | -1451.722805 |
| $^{Me}$**10** | 0 | -1294.014953 | -1293.445420 | -1291.664747 | -1294.023629 |
| **TS** $^{Me}$**10** | 1 (–223 $cm^{-1}$) | -1293.948847 | -1293.383066 | -1291.584952 | -1293.957621 |
| $^{Et}$**10** | 0 | -1451.240853 | -1450.564793 | -1448.619008 | -1451.249363 |
| **TS** $^{Et}$**10** | 1 (–159 $cm^{-1}$) | -1451.182306 | -1450.510629 | -1448.549238 | -1451.192234 |
| $^{Me}$**11** | 0 | -306.4344683 | -306.3074777 | -305.8922493 | -306.0133097 |
| $^{Et}$**11** | 0 | -385.0593026 | -384.8803367 | -384.3810485 | -384.6336912 |
| $^{Me}$**12** | 0 | -764.955858 | -764.667934 | -763.5699874 | -765.0180989 |
| **TS** $^{Me}$**12** | 1 (–146 $cm^{-1}$) | -764.9360313 | -764.6513463 | -763.5375165 | -764.9971882 |
| $^{Et}$**12** | 0 | -922.2035801 | -921.8097057 | -920.5478849 | -922.2634073 |
| **TS** $^{Et}$**12** | 1 (–149 $cm^{-1}$) | -922.1835069 | -921.7922878 | -920.5143034 | -922.2425731 |
| $^{Me}$**13** | 0 | -764.5261582 | -764.2524601 | -763.1347795 | -764.5333671 |
| **TS** $^{Me}$**13** | 1 (–292 $cm^{-1}$) | -764.4776008 | -764.20721 | -763.0758051 | -764.4872702 |
| $^{Et}$**13** | 0 | -921.7656588 | -921.3859613 | -920.1026274 | -921.7731259 |
| **TS** $^{Et}$**13** | 1 (–185 $cm^{-1}$) | -921.7190145 | -921.3431573 | -920.0462436 | -921.7288595 |
| $^{Me}$**14** | 0 | -835.9254664 | -835.5065928 | -834.4232875 | -835.9882303 |
| $^{Et}$**14** | 0 | -914.5422281 | -914.07058 | -912.9043271 | -914.6037547 |
| $^{Me}$**15** | 0 | -306.0039183 | -305.8911377 | -305.4623561 | -306.0133097 |
| $^{Et}$**15** | 0 | -384.6241219 | -384.4594675 | -383.946946 | -384.6336912 |

**Table S2**. Electronic ($\Delta E$) and Gibbs free energies ($\Delta G$). All energies are given in [Eh].

## XYZ Coordinates

**$^{Me}$4**

| | | | |
|---|---|---|---|
| C | 0.37100 | -1.69686 | 0.31719 |
| C | 0.40573 | -0.33384 | -0.05265 |
| N | -0.86465 | 0.16980 | 0.25356 |
| N | -0.91777 | -1.91587 | 0.81958 |
| C | -1.70224 | -0.78281 | 0.79292 |
| C | 1.48471 | -2.52356 | 0.14975 |
| C | 2.63779 | -1.94660 | -0.39975 |
| C | 2.67242 | -0.58831 | -0.76825 |
| C | 1.55519 | 0.24117 | -0.60032 |
| H | 1.46208 | -3.57265 | 0.43298 |
| H | 3.52360 | -2.56045 | -0.54438 |
| H | 3.58444 | -0.17441 | -1.19168 |
| H | 1.58605 | 1.28937 | -0.88602 |
| C | -1.38959 | -3.20184 | 1.32011 |
| H | -2.42427 | -3.07131 | 1.64199 |
| H | -0.77937 | -3.53379 | 2.16989 |
| H | -1.34319 | -3.96436 | 0.53202 |
| C | -1.26826 | 1.55331 | 0.03027 |
| H | -2.30486 | 1.65169 | 0.35735 |
| H | -1.19242 | 1.81138 | -1.03382 |
| H | -0.63430 | 2.23928 | 0.60669 |

**$^{Et}$4**

| | | | |
|---|---|---|---|
| C | 0.43576 | -1.73604 | 0.21966 |
| C | 0.49349 | -0.37677 | -0.16218 |
| N | -0.74723 | 0.16695 | 0.19894 |
| N | -0.83556 | -1.91325 | 0.78337 |
| C | -1.58242 | -0.75630 | 0.78751 |
| C | 1.51050 | -2.59997 | -0.00984 |
| C | 2.64667 | -2.06652 | -0.63179 |
| C | 2.70420 | -0.71200 | -1.01225 |
| C | 1.62749 | 0.15438 | -0.78351 |
| H | 1.47169 | -3.64630 | 0.28113 |
| H | 3.50136 | -2.71086 | -0.82343 |
| H | 3.60246 | -0.33068 | -1.49197 |
| H | 1.67746 | 1.19875 | -1.07978 |
| C | -1.31529 | -3.17240 | 1.36050 |
| H | -2.40502 | -3.09207 | 1.40111 |
| H | -1.05889 | -3.98899 | 0.67230 |
| C | -1.11325 | 1.57596 | 0.02728 |
| H | -2.20491 | 1.61457 | 0.07637 |
| H | -0.80557 | 1.89373 | -0.97797 |
| C | -0.48846 | 2.47933 | 1.09936 |
| H | -0.83128 | 2.17569 | 2.09479 |
| H | 0.60601 | 2.42322 | 1.08061 |
| H | -0.78077 | 3.52344 | 0.93335 |
| C | -0.73714 | -3.43554 | 2.75784 |
| H | -1.11550 | -4.38652 | 3.15232 |
| H | 0.35749 | -3.48626 | 2.73421 |
| H | -1.02926 | -2.63287 | 3.44413 |

**$^{Me}$7**

| | | | |
|---|---|---|---|
| N | -7.34590 | 8.11007 | 1.93654 |
| C | -6.62402 | 9.50787 | 3.96465 |
| C | -4.98245 | 9.03381 | 2.13983 |
| C | -7.10448 | 9.74319 | -0.87977 |
| C | -9.24940 | 10.45064 | 0.24482 |
| C | -8.10109 | 8.31224 | 0.88543 |
| C | -7.88628 | 9.76163 | 0.45776 |
| C | -6.46519 | 9.29809 | 2.45281 |
| C | -7.06937 | 10.44078 | 1.61055 |
| H | -9.11956 | 8.48146 | 3.54630 |
| H | -5.98189 | 10.33891 | 4.28114 |
| H | -7.65308 | 9.75881 | 4.23440 |
| H | -4.38115 | 9.87315 | 2.50957 |
| H | -4.62947 | 8.12425 | 2.63722 |
| H | -4.80158 | 8.93681 | 1.06596 |
| H | -7.65971 | 9.18171 | -1.63892 |
| H | -6.95332 | 10.76893 | -1.24114 |
| H | -6.12061 | 9.27304 | -0.76785 |
| H | -9.10839 | 11.50197 | -0.04127 |
| H | -9.81688 | 9.94477 | -0.54400 |
| H | -9.84988 | 10.42312 | 1.16258 |
| H | -7.74237 | 11.04087 | 2.23423 |
| H | -6.29168 | 11.11164 | 1.22990 |
| C | -7.28751 | 6.82041 | 2.60421 |
| C | -8.18128 | 6.56656 | 3.66880 |
| C | -6.37299 | 5.84347 | 2.15290 |
| C | -8.06416 | 5.34557 | 4.34955 |
| C | -6.29364 | 4.63826 | 2.86859 |
| C | -7.11163 | 4.39848 | 3.97224 |
| H | -8.73870 | 5.12573 | 5.17300 |
| H | -5.59686 | 3.86991 | 2.54343 |
| H | -7.02980 | 3.46061 | 4.51789 |
| C | -5.59888 | 5.99875 | 0.84670 |
| H | -5.61657 | 7.05205 | 0.56391 |
| C | -6.33757 | 5.23238 | -0.27713 |
| C | -4.12309 | 5.56622 | 0.94809 |
| H | -3.60342 | 6.09561 | 1.75556 |
| H | -4.02512 | 4.49008 | 1.13496 |
| H | -3.60243 | 5.78300 | 0.00708 |
| H | -6.37767 | 4.15805 | -0.05678 |
| H | -5.81942 | 5.36682 | -1.23563 |
| H | -7.36187 | 5.60683 | -0.37935 |
| C | -9.34090 | 7.50699 | 3.98738 |
| H | -6.32199 | 8.61703 | 4.52637 |
| C | -9.56928 | 7.71760 | 5.49673 |
| C | -10.62085 | 6.99122 | 3.28597 |
| H | -10.45765 | 6.91869 | 2.20503 |

| | | | |
|---|---|---|---|
| H | -10.89925 | 5.99934 | 3.66414 |
| H | -11.45966 | 7.67575 | 3.46790 |
| H | -9.89714 | 6.79590 | 5.99212 |
| H | -10.35189 | 8.46955 | 5.65710 |
| H | -8.65597 | 8.06133 | 5.99656 |

**$^{Et}$7**

| | | | |
|---|---|---|---|
| C | -7.18799 | 8.43224 | 0.70045 |
| C | -7.24397 | 6.90552 | 0.48480 |
| C | -5.82223 | 8.92194 | 0.10654 |
| H | -7.22341 | 8.65450 | 1.77359 |
| H | -8.04881 | 8.92781 | 0.24071 |
| N | -5.73847 | 6.63995 | 0.16084 |
| C | -4.96011 | 7.67199 | -0.04898 |
| C | -5.98803 | 9.53688 | -1.31675 |
| H | -6.50185 | 8.80311 | -1.95249 |
| H | -4.99160 | 9.66264 | -1.75592 |
| C | -5.12505 | 9.90471 | 1.09044 |
| H | -4.96077 | 9.36166 | 2.03257 |
| H | -5.82667 | 10.71722 | 1.32912 |
| C | -7.70168 | 6.13362 | 1.73008 |
| H | -7.14626 | 6.43506 | 2.62189 |
| H | -7.58818 | 5.05223 | 1.59555 |
| H | -8.76358 | 6.34078 | 1.91032 |
| C | -8.12663 | 6.49528 | -0.70670 |
| H | -7.88403 | 7.06251 | -1.60943 |
| H | -9.17768 | 6.68711 | -0.45921 |
| H | -8.02369 | 5.42736 | -0.92656 |
| C | -5.23970 | 5.27696 | 0.08545 |
| C | -4.73279 | 4.67403 | 1.25851 |
| C | -5.23564 | 4.60559 | -1.15678 |
| C | -4.32111 | 3.33504 | 1.18471 |
| C | -4.81496 | 3.26631 | -1.17763 |
| C | -4.38565 | 2.62625 | -0.01543 |
| H | -3.92839 | 2.84665 | 2.07276 |
| H | -4.80352 | 2.72541 | -2.12045 |
| H | -4.07028 | 1.58542 | -0.05113 |
| C | -4.48974 | 5.47666 | 2.53423 |
| H | -5.09225 | 6.38628 | 2.48399 |
| C | -3.01156 | 5.93466 | 2.57219 |
| C | -4.88285 | 4.72654 | 3.82146 |
| H | -5.92394 | 4.38461 | 3.78421 |
| H | -4.24697 | 3.84993 | 3.99371 |
| H | -4.76955 | 5.38660 | 4.69043 |
| H | -2.33668 | 5.06992 | 2.60507 |
| H | -2.82394 | 6.55067 | 3.46136 |
| H | -2.77617 | 6.52674 | 1.68095 |
| C | -5.52076 | 5.32965 | -2.46972 |
| H | -6.03126 | 6.26534 | -2.23831 |
| C | -6.42088 | 4.53167 | -3.43294 |
| C | -4.17969 | 5.71819 | -3.13794 |
| H | -3.58842 | 6.34478 | -2.46138 |
| H | -3.59418 | 4.82455 | -3.38878 |
| H | -4.36235 | 6.27960 | -4.06354 |
| H | -5.93037 | 3.61708 | -3.78726 |
| H | -6.65739 | 5.13831 | -4.31593 |
| H | -7.36438 | 4.24268 | -2.95475 |
| C | -3.78811 | 10.48744 | 0.60898 |
| H | -3.10278 | 9.68420 | 0.31989 |
| H | -3.91820 | 11.14832 | -0.25634 |
| H | -3.31821 | 11.07812 | 1.40532 |
| C | -6.75155 | 10.87013 | -1.36696 |
| H | -7.75766 | 10.78295 | -0.93806 |
| H | -6.22575 | 11.66055 | -0.81945 |
| H | -6.86419 | 11.20609 | -2.40513 |

**$^{Me}$9**

| | | | |
|---|---|---|---|
| C | 0.18816 | 10.12280 | 0.59045 |
| C | 0.20224 | 10.69823 | 1.87940 |
| C | 1.31740 | 9.50021 | 0.05620 |
| C | 2.46034 | 9.47827 | 0.86030 |
| C | 2.47721 | 10.05226 | 2.14493 |
| C | 1.34476 | 10.67377 | 2.68119 |
| H | -0.72328 | 10.16575 | 0.00088 |
| H | -0.69858 | 11.17351 | 2.25723 |
| H | 1.30180 | 9.05671 | -0.93442 |
| H | 1.34217 | 11.12105 | 3.67019 |
| N | 3.73181 | 8.93065 | 0.64710 |
| N | 3.76518 | 9.82924 | 2.65450 |
| C | 4.51913 | 9.15993 | 1.73497 |
| C | 5.97159 | 8.77102 | 2.00050 |
| N | 6.14954 | 7.32517 | 2.05881 |
| C | 7.05378 | 9.32465 | 0.98628 |
| H | 6.18209 | 9.22978 | 2.97452 |
| C | 7.50410 | 8.04438 | 0.23056 |
| C | 7.22653 | 6.80948 | 1.13277 |
| H | 8.56440 | 8.10162 | -0.03514 |
| H | 6.95851 | 7.95173 | -0.71490 |
| C | 6.72985 | 5.60818 | 0.30251 |
| H | 5.81601 | 5.83252 | -0.25420 |
| H | 6.53075 | 4.74884 | 0.94998 |
| H | 7.50007 | 5.30973 | -0.41749 |
| C | 8.50320 | 6.33661 | 1.86347 |
| H | 9.18941 | 5.88606 | 1.13791 |
| H | 8.25735 | 5.57242 | 2.60675 |
| H | 9.03613 | 7.14788 | 2.36099 |
| C | 6.54220 | 10.42512 | 0.03561 |
| H | 5.76758 | 10.07812 | -0.65138 |
| H | 7.37321 | 10.79278 | -0.57644 |
| H | 6.14685 | 11.28285 | 0.59465 |
| C | 8.22360 | 9.93746 | 1.79413 |
| H | 8.66582 | 9.22849 | 2.49627 |
| H | 7.88963 | 10.81401 | 2.36267 |

| | | | |
|---|---|---|---|
| H | 9.01420 | 10.26330 | 1.10920 |
| C | 4.04946 | 8.19167 | -0.57752 |
| H | 5.03012 | 7.73983 | -0.48957 |
| H | 4.02636 | 8.86972 | -1.43611 |
| H | 3.30176 | 7.40561 | -0.71514 |
| C | 4.17978 | 10.19510 | 4.01965 |
| H | 4.53570 | 9.30848 | 4.54819 |
| H | 3.30808 | 10.59089 | 4.54088 |
| H | 4.95758 | 10.96256 | 3.99756 |
| C | 5.68375 | 6.64206 | 3.25266 |
| C | 6.32566 | 6.82372 | 4.51650 |
| C | 4.51612 | 5.83095 | 3.17720 |
| C | 5.78854 | 6.19114 | 5.64815 |
| C | 4.03834 | 5.20049 | 4.33670 |
| C | 4.66195 | 5.37695 | 5.56747 |
| H | 6.27581 | 6.32692 | 6.61046 |
| H | 3.15349 | 4.57201 | 4.27357 |
| H | 4.27438 | 4.88563 | 6.45692 |
| C | 7.59016 | 7.65570 | 4.72936 |
| H | 7.90926 | 8.03026 | 3.75911 |
| C | 8.74705 | 6.80156 | 5.30080 |
| C | 7.35748 | 8.88052 | 5.64374 |
| H | 6.61842 | 9.57238 | 5.22752 |
| H | 7.00761 | 8.57641 | 6.63682 |
| H | 8.29320 | 9.43679 | 5.77515 |
| H | 8.53976 | 6.49650 | 6.33260 |
| H | 9.67804 | 7.38122 | 5.30739 |
| H | 8.91171 | 5.89458 | 4.71240 |
| C | 3.70992 | 5.64511 | 1.89666 |
| H | 4.22163 | 6.20816 | 1.11626 |
| C | 2.28221 | 6.21911 | 2.05381 |
| C | 3.63991 | 4.16823 | 1.44991 |
| H | 4.63693 | 3.73074 | 1.34221 |
| H | 3.08680 | 3.56134 | 2.17595 |
| H | 3.12340 | 4.08304 | 0.48558 |
| H | 1.68913 | 5.61526 | 2.74982 |
| H | 1.75389 | 6.22163 | 1.09178 |
| H | 2.29537 | 7.24242 | 2.44258 |

**TS $^{Me}$9**

| | | | |
|---|---|---|---|
| C | -0.75890 | 9.41103 | -0.18750 |
| C | -0.79462 | 10.25660 | 0.93882 |
| C | 0.44630 | 8.88608 | -0.66896 |
| C | 1.61134 | 9.23611 | 0.01852 |
| C | 1.57583 | 10.08367 | 1.14405 |
| C | 0.37371 | 10.60917 | 1.62477 |
| H | -1.68743 | 9.16154 | -0.69405 |
| H | -1.75009 | 10.64448 | 1.28175 |
| H | 0.46776 | 8.23542 | -1.53880 |
| H | 0.34022 | 11.26294 | 2.49185 |
| N | 2.96297 | 8.90359 | -0.16137 |
| N | 2.90793 | 10.20336 | 1.56870 |
| C | 3.77546 | 9.47806 | 0.78769 |
| C | 6.70250 | 8.72276 | 2.68814 |
| N | 6.64078 | 7.43531 | 2.57964 |
| C | 7.54145 | 9.40096 | 1.64969 |
| H | 6.26079 | 9.21063 | 3.55447 |
| C | 7.64624 | 8.27625 | 0.57609 |
| C | 7.33613 | 6.92696 | 1.28396 |
| H | 8.63072 | 8.25636 | 0.10135 |
| H | 6.89531 | 8.46337 | -0.19663 |
| C | 6.36656 | 6.05035 | 0.48942 |
| H | 5.44719 | 6.58651 | 0.25151 |
| H | 6.11967 | 5.13380 | 1.03339 |
| H | 6.85304 | 5.76512 | -0.44979 |
| C | 8.58776 | 6.11388 | 1.64696 |
| H | 9.01993 | 5.72404 | 0.71948 |
| H | 8.33407 | 5.26120 | 2.28374 |
| H | 9.35145 | 6.71365 | 2.14585 |
| C | 6.94357 | 10.71135 | 1.10239 |
| H | 5.95250 | 10.52609 | 0.67800 |
| H | 7.61299 | 11.11357 | 0.33351 |
| H | 6.85956 | 11.46533 | 1.89497 |
| C | 8.91750 | 9.72362 | 2.31957 |
| H | 9.43198 | 8.82771 | 2.67624 |
| H | 8.79449 | 10.41176 | 3.16319 |
| H | 9.55260 | 10.21222 | 1.57305 |
| C | 3.44618 | 8.07552 | -1.26134 |
| H | 4.53661 | 8.08068 | -1.23758 |
| H | 3.10792 | 8.48389 | -2.22045 |
| H | 3.08059 | 7.04568 | -1.16721 |
| C | 3.31222 | 11.00803 | 2.71560 |
| H | 4.39757 | 10.95069 | 2.80658 |
| H | 2.84525 | 10.63396 | 3.63471 |
| H | 3.02024 | 12.05490 | 2.57207 |
| C | 6.13272 | 6.52478 | 3.60891 |
| C | 7.01001 | 6.16875 | 4.66346 |
| C | 4.82125 | 6.01170 | 3.50175 |
| C | 6.56465 | 5.18988 | 5.56342 |
| C | 4.44101 | 5.02858 | 4.42854 |
| C | 5.30739 | 4.60179 | 5.43235 |
| H | 7.21130 | 4.89101 | 6.38312 |
| H | 3.43979 | 4.61066 | 4.37302 |
| H | 4.99134 | 3.83375 | 6.13403 |
| C | 8.34430 | 6.86490 | 4.92222 |
| H | 8.63070 | 7.41499 | 4.02434 |
| C | 9.49525 | 5.88702 | 5.23622 |
| C | 8.17973 | 7.90752 | 6.05513 |
| H | 7.39397 | 8.63654 | 5.82121 |
| H | 7.90576 | 7.41969 | 6.99756 |
| H | 9.11811 | 8.45198 | 6.21323 |
| H | 9.34115 | 5.37189 | 6.19044 |
| H | 10.44128 | 6.43542 | 5.31139 |
| H | 9.60164 | 5.12558 | 4.45602 |

| | | | |
|---|---|---|---|
| C | 3.77195 | 6.57874 | 2.55088 |
| H | 4.25229 | 7.29380 | 1.87571 |
| C | 2.73117 | 7.37876 | 3.37306 |
| C | 3.06290 | 5.50547 | 1.70005 |
| H | 3.76991 | 4.91292 | 1.11089 |
| H | 2.48613 | 4.81358 | 2.32409 |
| H | 2.35815 | 5.98661 | 1.01210 |
| H | 2.20781 | 6.72788 | 4.08252 |
| H | 1.98501 | 7.82702 | 2.70970 |
| H | 3.21100 | 8.17988 | 3.94658 |

**$^{Et}$9**

| | | | |
|---|---|---|---|
| C | -7.21227 | 8.44782 | 0.67900 |
| C | -7.26284 | 6.90559 | 0.48630 |
| C | -5.85319 | 8.95754 | 0.09598 |
| H | -7.26556 | 8.68734 | 1.74555 |
| H | -8.06505 | 8.92622 | 0.19278 |
| N | -5.77078 | 6.60924 | 0.16054 |
| C | -5.09242 | 7.68565 | -0.04586 |
| C | -5.99845 | 9.58881 | -1.33402 |
| H | -6.53600 | 8.87471 | -1.97065 |
| H | -5.00163 | 9.70439 | -1.77703 |
| C | -5.12420 | 9.91125 | 1.09579 |
| H | -5.01513 | 9.37827 | 2.05015 |
| H | -5.80807 | 10.74553 | 1.29381 |
| C | -7.70120 | 6.14949 | 1.74379 |
| H | -7.14628 | 6.46538 | 2.62962 |
| H | -7.59226 | 5.06764 | 1.61915 |
| H | -8.76116 | 6.36359 | 1.91687 |
| C | -8.12922 | 6.47318 | -0.70648 |
| H | -7.88401 | 7.02319 | -1.61849 |
| H | -9.17555 | 6.67902 | -0.45811 |
| H | -8.03416 | 5.40101 | -0.90018 |
| H | -4.04126 | 7.61124 | -0.31594 |
| C | -5.20808 | 5.26238 | 0.07267 |
| C | -4.68726 | 4.68864 | 1.25422 |
| C | -5.18846 | 4.61285 | -1.18104 |
| C | -4.22379 | 3.36812 | 1.16651 |
| C | -4.71292 | 3.29249 | -1.20080 |
| C | -4.25934 | 2.66821 | -0.03970 |
| H | -3.81528 | 2.88844 | 2.05113 |
| H | -4.68232 | 2.75447 | -2.14385 |
| H | -3.90296 | 1.64192 | -0.08069 |
| C | -4.49172 | 5.47952 | 2.54645 |
| H | -5.08765 | 6.39558 | 2.49069 |
| C | -3.01102 | 5.91778 | 2.66608 |
| C | -4.94766 | 4.71289 | 3.80444 |
| H | -5.98612 | 4.37538 | 3.71663 |
| H | -4.32269 | 3.83248 | 3.98884 |
| H | -4.86934 | 5.35888 | 4.68623 |
| H | -2.34983 | 5.04630 | 2.73201 |
| H | -2.86415 | 6.52658 | 3.56579 |
| H | -2.69413 | 6.50712 | 1.79629 |
| C | -5.52778 | 5.31173 | -2.49568 |
| H | -6.02365 | 6.25972 | -2.27141 |
| C | -6.48432 | 4.49399 | -3.38787 |
| C | -4.22183 | 5.65791 | -3.25303 |
| H | -3.55294 | 6.27507 | -2.64022 |
| H | -3.67401 | 4.74891 | -3.52592 |
| H | -4.44947 | 6.20751 | -4.17378 |
| H | -6.01524 | 3.56817 | -3.73814 |
| H | -6.76139 | 5.07633 | -4.27390 |
| H | -7.40250 | 4.22315 | -2.85515 |
| C | -3.75923 | 10.44869 | 0.64302 |
| H | -3.03758 | 9.64508 | 0.45028 |
| H | -3.83535 | 11.05677 | -0.26426 |
| H | -3.33147 | 11.08244 | 1.42703 |
| C | -6.72837 | 10.94022 | -1.34744 |
| H | -7.72568 | 10.87174 | -0.89819 |
| H | -6.16881 | 11.71395 | -0.81245 |
| H | -6.85430 | 11.27852 | -2.38150 |

**TS $^{Et}$9**

| | | | |
|---|---|---|---|
| C | 13.45992 | 5.60759 | 2.13355 |
| C | 14.14220 | 5.64310 | 0.90144 |
| C | 12.29528 | 4.85026 | 2.29954 |
| C | 11.83867 | 4.12858 | 1.19247 |
| C | 12.52674 | 4.15524 | -0.03766 |
| C | 13.68890 | 4.91524 | -0.20416 |
| H | 13.84512 | 6.18224 | 2.97170 |
| H | 15.04134 | 6.24647 | 0.80864 |
| H | 11.77253 | 4.83090 | 3.25165 |
| H | 14.22380 | 4.94516 | -1.14893 |
| N | 10.73287 | 3.28632 | 0.98912 |
| N | 11.79101 | 3.32565 | -0.90074 |
| C | 10.67847 | 2.79139 | -0.29209 |
| C | 8.04412 | 2.20790 | -2.91075 |
| N | 7.43995 | 1.24242 | -2.29834 |
| C | 7.50260 | 3.57292 | -2.62762 |
| H | 8.81313 | 1.97583 | -3.64335 |
| C | 6.64026 | 3.29297 | -1.35995 |
| C | 6.37000 | 1.76459 | -1.30036 |
| H | 5.70397 | 3.85535 | -1.36867 |
| H | 7.20798 | 3.60142 | -0.47809 |
| C | 6.62277 | 1.17802 | 0.08939 |
| H | 7.62585 | 1.41844 | 0.44455 |
| H | 6.48679 | 0.09277 | 0.09669 |
| H | 5.89590 | 1.61567 | 0.78231 |
| C | 4.96858 | 1.36495 | -1.78588 |
| H | 4.87808 | 0.27881 | -1.88101 |
| H | 4.70681 | 1.82723 | -2.73998 |
| H | 4.24126 | 1.69960 | -1.03893 |
| C | 8.60575 | 4.63108 | -2.35433 |
| H | 8.10209 | 5.53108 | -1.98057 |

| | | | |
|---|---|---|---|
| H | 9.22820 | 4.25314 | -1.53647 |
| C | 6.62412 | 3.96731 | -3.87626 |
| H | 5.83718 | 3.21566 | -4.00165 |
| H | 7.24326 | 3.91506 | -4.77996 |
| C | 9.74648 | 2.97505 | 2.02968 |
| H | 10.29046 | 2.75189 | 2.95597 |
| H | 9.24412 | 2.05622 | 1.71692 |
| C | 12.20990 | 2.99728 | -2.26790 |
| H | 12.39136 | 3.93372 | -2.81095 |
| H | 11.35462 | 2.49910 | -2.73295 |
| C | 7.60168 | -0.18010 | -2.61084 |
| C | 6.87933 | -0.69900 | -3.71385 |
| C | 8.43629 | -0.97886 | -1.79916 |
| C | 6.94139 | -2.08439 | -3.92300 |
| C | 8.44617 | -2.35880 | -2.05576 |
| C | 7.69146 | -2.91163 | -3.08805 |
| H | 6.39940 | -2.51877 | -4.75792 |
| H | 9.07611 | -3.00239 | -1.44812 |
| H | 7.71163 | -3.98448 | -3.26363 |
| C | 6.13705 | 0.17288 | -4.72410 |
| H | 6.00367 | 1.16792 | -4.29589 |
| C | 4.73075 | -0.35737 | -5.07225 |
| C | 6.99533 | 0.34562 | -6.00104 |
| H | 7.98228 | 0.76488 | -5.76934 |
| H | 7.15571 | -0.61839 | -6.49717 |
| H | 6.49516 | 1.01523 | -6.71069 |
| H | 4.77837 | -1.30937 | -5.61177 |
| H | 4.21078 | 0.35849 | -5.71932 |
| H | 4.12410 | -0.51040 | -4.17312 |
| C | 9.41817 | -0.40156 | -0.78721 |
| H | 9.24815 | 0.67385 | -0.68006 |
| C | 10.85546 | -0.53681 | -1.34298 |
| C | 9.32133 | -1.05515 | 0.60635 |
| H | 8.30506 | -1.01396 | 1.01177 |
| H | 9.62735 | -2.10734 | 0.58205 |
| H | 9.98919 | -0.53627 | 1.30411 |
| H | 11.14237 | -1.58873 | -1.45738 |
| H | 11.55920 | -0.05457 | -0.65702 |
| H | 10.94897 | -0.05283 | -2.32200 |
| C | 5.97984 | 5.35776 | -3.77095 |
| H | 5.35907 | 5.45371 | -2.87295 |
| H | 6.72534 | 6.15828 | -3.75325 |
| H | 5.33254 | 5.52615 | -4.63867 |
| C | 9.49303 | 4.99704 | -3.55276 |
| H | 10.28275 | 5.68487 | -3.23183 |
| H | 9.98778 | 4.11891 | -3.98456 |
| H | 8.93337 | 5.49176 | -4.35344 |
| C | 13.45102 | 2.09721 | -2.31694 |
| H | 13.26867 | 1.15805 | -1.78597 |
| H | 13.70202 | 1.86466 | -3.35841 |
| H | 14.31856 | 2.58413 | -1.86076 |
| C | 8.73646 | 4.10570 | 2.25881 |
| H | 8.04036 | 3.83458 | 3.06107 |
| H | 9.23775 | 5.03702 | 2.54237 |
| H | 8.15634 | 4.29778 | 1.34947 |

**$^{Me}$10**

| | | | |
|---|---|---|---|
| C | -7.82567 | 1.77512 | 1.57759 |
| C | -6.59324 | 1.24080 | 1.97163 |
| C | -7.89060 | 2.81872 | 0.63392 |
| C | -5.45583 | 2.79370 | 0.53439 |
| C | -5.38711 | 1.73954 | 1.44600 |
| H | -4.43066 | 1.31664 | 1.74430 |
| H | -8.74627 | 1.37939 | 1.99991 |
| H | -6.56388 | 0.43069 | 2.69680 |
| C | -6.69859 | 3.32675 | 0.12721 |
| H | -8.85088 | 3.20856 | 0.30543 |
| N | -6.49651 | 4.31353 | -0.89513 |
| C | -5.05130 | 4.57711 | -0.83258 |
| N | -4.42861 | 3.45158 | -0.16333 |
| C | -7.11802 | 3.88884 | -2.17858 |
| H | -8.18799 | 3.74006 | -2.00758 |
| H | -6.69006 | 2.94163 | -2.54637 |
| H | -6.99725 | 4.65958 | -2.93415 |
| C | -3.34358 | 2.65860 | -0.75453 |
| H | -3.64549 | 1.60427 | -0.83230 |
| H | -2.42183 | 2.70763 | -0.15685 |
| H | -3.12496 | 3.03539 | -1.75760 |
| C | -4.44479 | 5.79521 | -0.91881 |
| N | -4.99433 | 6.94877 | -1.51883 |
| C | -4.16229 | 8.18602 | -1.29090 |
| C | -3.20835 | 7.70493 | -0.18199 |
| C | -3.08043 | 6.15901 | -0.29208 |
| H | -3.64602 | 7.95230 | 0.79241 |
| H | -2.23242 | 8.19856 | -0.24133 |
| C | -5.00278 | 9.37751 | -0.79946 |
| H | -5.55983 | 9.12991 | 0.10746 |
| H | -5.70626 | 9.70877 | -1.56906 |
| H | -4.33612 | 10.21848 | -0.57250 |
| C | -3.41465 | 8.65415 | -2.56108 |
| H | -2.86715 | 9.57774 | -2.33959 |
| H | -4.12452 | 8.87078 | -3.36603 |
| H | -2.69574 | 7.91835 | -2.92347 |
| C | -1.86053 | 5.77821 | -1.17010 |
| H | -1.94381 | 6.16707 | -2.18812 |
| H | -1.73900 | 4.69494 | -1.23540 |
| H | -0.94459 | 6.19292 | -0.72801 |
| C | -2.87136 | 5.59020 | 1.13021 |
| H | -2.04236 | 6.12707 | 1.61048 |
| H | -3.77143 | 5.72969 | 1.73891 |
| H | -2.62915 | 4.52643 | 1.12820 |
| C | -5.99176 | 6.92248 | -2.55574 |
| C | -7.32375 | 7.33056 | -2.27342 |
| C | -8.25873 | 7.34851 | -3.32031 |

| | | | |
|---|---|---|---|
| C | -7.91554 | 6.95453 | -4.61153 |
| C | -6.61897 | 6.51354 | -4.87146 |
| C | -5.64240 | 6.48388 | -3.86555 |
| H | -9.28049 | 7.65768 | -3.11266 |
| H | -8.65771 | 6.97444 | -5.40704 |
| H | -6.36090 | 6.17704 | -5.87298 |
| C | -7.81644 | 7.67478 | -0.86803 |
| C | -8.44253 | 9.08593 | -0.78949 |
| H | -7.77884 | 9.85878 | -1.18836 |
| H | -8.67411 | 9.33855 | 0.25296 |
| H | -9.38193 | 9.13064 | -1.35449 |
| C | -8.83512 | 6.62873 | -0.35816 |
| H | -6.95297 | 7.62969 | -0.20018 |
| H | -9.72084 | 6.58844 | -1.00470 |
| H | -9.16909 | 6.89300 | 0.65347 |
| H | -8.37344 | 5.64054 | -0.32346 |
| C | -4.26809 | 5.91540 | -4.21615 |
| C | -4.32941 | 4.38913 | -4.45678 |
| H | -4.69268 | 3.86566 | -3.56891 |
| H | -3.32940 | 4.00461 | -4.69556 |
| H | -4.99417 | 4.14559 | -5.29504 |
| C | -3.62785 | 6.61735 | -5.43406 |
| H | -3.61742 | 6.07075 | -3.35683 |
| H | -4.17826 | 6.39857 | -6.35694 |
| H | -2.59809 | 6.26463 | -5.57435 |
| H | -3.60336 | 7.70447 | -5.30917 |

**TS $^{Me}$10**

| | | | |
|---|---|---|---|
| C | -6.54585 | 0.13604 | 0.48395 |
| C | -5.17444 | -0.09149 | 0.69120 |
| C | -7.01113 | 1.32078 | -0.10638 |
| C | -4.68109 | 2.04994 | -0.25718 |
| C | -4.21736 | 0.86747 | 0.32078 |
| H | -3.15657 | 0.69161 | 0.47961 |
| H | -7.26345 | -0.62514 | 0.78123 |
| H | -4.84815 | -1.02611 | 1.14092 |
| C | -6.05955 | 2.27749 | -0.47450 |
| H | -8.07235 | 1.47970 | -0.27696 |
| N | -6.15523 | 3.51760 | -1.10194 |
| C | -4.91129 | 4.12305 | -1.27198 |
| N | -4.02196 | 3.17345 | -0.76843 |
| C | -7.39990 | 4.21666 | -1.36601 |
| H | -7.30438 | 5.20685 | -0.90065 |
| H | -8.23517 | 3.66189 | -0.93243 |
| H | -7.56469 | 4.34965 | -2.43978 |
| C | -2.59882 | 3.15479 | -1.08147 |
| H | -2.36279 | 2.26883 | -1.68640 |
| H | -1.98589 | 3.13494 | -0.17280 |
| H | -2.36425 | 4.05156 | -1.65653 |
| C | -5.11657 | 6.09117 | -0.60778 |
| N | -5.06359 | 6.99980 | -1.60240 |
| C | -3.86981 | 7.96359 | -1.56416 |
| C | -3.62217 | 7.97684 | -0.04245 |
| C | -4.14894 | 6.59954 | 0.49336 |
| H | -4.19550 | 8.79535 | 0.41033 |
| H | -2.56644 | 8.14348 | 0.19903 |
| C | -4.22664 | 9.33649 | -2.14120 |
| H | -5.04396 | 9.80572 | -1.58718 |
| H | -4.52318 | 9.25907 | -3.19359 |
| H | -3.35436 | 9.99869 | -2.08409 |
| C | -2.64928 | 7.38441 | -2.30986 |
| H | -1.75292 | 7.96140 | -2.05150 |
| H | -2.77546 | 7.42966 | -3.39321 |
| H | -2.47703 | 6.34150 | -2.02535 |
| C | -2.98611 | 5.67470 | 0.89318 |
| H | -2.27260 | 5.54027 | 0.07712 |
| H | -3.35345 | 4.69243 | 1.20392 |
| H | -2.44346 | 6.11675 | 1.73938 |
| C | -5.02476 | 6.81733 | 1.75600 |
| H | -4.43581 | 7.30505 | 2.54620 |
| H | -5.89112 | 7.44848 | 1.53408 |
| H | -5.39610 | 5.85880 | 2.13573 |
| C | -6.12703 | 7.07375 | -2.58049 |
| C | -7.30983 | 7.77472 | -2.22518 |
| C | -8.38026 | 7.79133 | -3.12958 |
| C | -8.29473 | 7.14742 | -4.36426 |
| C | -7.12628 | 6.47130 | -4.70512 |
| C | -6.03065 | 6.41092 | -3.82719 |
| H | -9.29380 | 8.31924 | -2.86537 |
| H | -9.13510 | 7.17333 | -5.05518 |
| H | -7.06290 | 5.96729 | -5.66672 |
| C | -7.46763 | 8.50214 | -0.89099 |
| C | -7.88111 | 9.97880 | -1.08148 |
| H | -7.20115 | 10.50114 | -1.76412 |
| H | -7.86991 | 10.50204 | -0.11692 |
| H | -8.89446 | 10.06438 | -1.49210 |
| C | -8.46493 | 7.77656 | 0.03977 |
| H | -6.49638 | 8.49220 | -0.39205 |
| H | -9.46030 | 7.71782 | -0.41845 |
| H | -8.56179 | 8.31578 | 0.99099 |
| H | -8.12506 | 6.75985 | 0.25889 |
| C | -4.79082 | 5.63771 | -4.26464 |
| C | -5.11294 | 4.17999 | -4.66002 |
| H | -5.59310 | 3.64994 | -3.83295 |
| H | -4.18595 | 3.64696 | -4.90820 |
| H | -5.76887 | 4.13066 | -5.53812 |
| C | -4.07915 | 6.35811 | -5.43378 |
| H | -4.12193 | 5.58456 | -3.40412 |
| H | -4.69794 | 6.33633 | -6.33990 |
| H | -3.12470 | 5.86871 | -5.66709 |
| H | -3.87821 | 7.41000 | -5.20125 |

**$^{Et}$10**

| | | | |
|---|---|---|---|
| C | -0.73223 | 4.20081 | 1.52914 |

| | | | |
|---|---|---|---|
| C | -1.55604 | 3.18459 | 1.02949 |
| C | -1.20397 | 2.46918 | -0.12947 |
| C | 0.00314 | 2.78002 | -0.75947 |
| C | 0.83114 | 3.80788 | -0.25430 |
| C | 0.47289 | 4.53041 | 0.88053 |
| N | 1.94882 | 3.96818 | -1.11445 |
| N | 0.56474 | 2.24614 | -1.94208 |
| C | 1.93351 | 2.80048 | -1.98316 |
| C | 3.09488 | 2.10530 | -2.20385 |
| C | 4.48771 | 2.46128 | -1.60125 |
| N | 3.23613 | 0.93332 | -2.97704 |
| C | 4.64118 | 0.38940 | -2.99055 |
| C | 5.20845 | 1.08957 | -1.75533 |
| H | 6.29638 | 1.18597 | -1.78724 |
| H | 4.96095 | 0.47964 | -0.87849 |
| H | -1.02470 | 4.74341 | 2.42499 |
| H | -2.48510 | 2.94339 | 1.54114 |
| H | 1.10298 | 5.33505 | 1.25257 |
| H | -1.86365 | 1.70190 | -0.52656 |
| C | 4.69126 | -1.14002 | -2.82857 |
| H | 4.23974 | -1.46332 | -1.88876 |
| H | 5.73861 | -1.46424 | -2.82983 |
| H | 4.18485 | -1.64486 | -3.65772 |
| C | 5.41748 | 0.72537 | -4.28669 |
| H | 6.43030 | 0.31127 | -4.21739 |
| H | 5.50480 | 1.79781 | -4.46378 |
| H | 4.93101 | 0.26867 | -5.15406 |
| C | 5.19616 | 3.59445 | -2.41031 |
| H | 4.92193 | 3.51134 | -3.46784 |
| H | 4.78459 | 4.54958 | -2.07653 |
| C | 4.45982 | 2.76546 | -0.05101 |
| H | 5.24751 | 2.14869 | 0.40304 |
| H | 3.51277 | 2.37954 | 0.34178 |
| C | 2.14981 | 5.33200 | -1.67376 |
| H | 3.02292 | 5.28887 | -2.32752 |
| H | 2.41146 | 5.98890 | -0.83424 |
| C | -0.37215 | 2.03056 | -3.07475 |
| H | -1.00491 | 1.17559 | -2.80617 |
| H | 0.20823 | 1.71801 | -3.93560 |
| C | 2.26331 | 0.42811 | -3.90423 |
| C | 2.11431 | 1.03676 | -5.18175 |
| C | 1.45785 | -0.68454 | -3.54036 |
| C | 1.18719 | 0.49177 | -6.08254 |
| C | 0.54619 | -1.18919 | -4.47985 |
| C | 0.41287 | -0.61694 | -5.74347 |
| H | 1.05972 | 0.95258 | -7.05934 |
| H | -0.08078 | -2.03594 | -4.21023 |
| H | -0.30128 | -1.02406 | -6.45643 |
| C | 2.85240 | 2.31249 | -5.58379 |
| H | 3.60409 | 2.51430 | -4.82100 |
| C | 1.89875 | 3.52847 | -5.59387 |
| C | 3.57052 | 2.18441 | -6.94433 |
| H | 4.22711 | 1.30880 | -6.97636 |
| H | 2.85348 | 2.09529 | -7.76931 |
| H | 4.18055 | 3.07656 | -7.13398 |
| H | 1.07896 | 3.38831 | -6.30928 |
| H | 2.44520 | 4.43765 | -5.87558 |
| H | 1.47027 | 3.68605 | -4.60178 |
| C | 1.49585 | -1.32128 | -2.15058 |
| H | 2.31099 | -0.84747 | -1.59847 |
| C | 1.75387 | -2.84418 | -2.21366 |
| C | 0.20114 | -1.04459 | -1.35277 |
| H | 0.08222 | 0.02601 | -1.17680 |
| H | -0.68253 | -1.41970 | -1.88454 |
| H | 0.24677 | -1.55028 | -0.37987 |
| H | 0.89592 | -3.37172 | -2.64847 |
| H | 1.90576 | -3.24288 | -1.20274 |
| H | 2.63467 | -3.08963 | -2.81479 |
| C | 4.67506 | 4.19636 | 0.46622 |
| H | 5.65493 | 4.59850 | 0.18408 |
| H | 3.90795 | 4.88669 | 0.11847 |
| H | 4.63533 | 4.18682 | 1.56310 |
| C | 6.72991 | 3.65831 | -2.29408 |
| H | 7.21854 | 2.83885 | -2.83275 |
| H | 7.10240 | 4.59749 | -2.72174 |
| H | 7.06398 | 3.61445 | -1.25095 |
| C | -1.26754 | 3.22018 | -3.45596 |
| H | -1.99886 | 2.89295 | -4.20659 |
| H | -1.81815 | 3.60895 | -2.59299 |
| H | -0.68824 | 4.03921 | -3.88939 |
| C | 0.95864 | 5.93227 | -2.43427 |
| H | 1.17152 | 6.97774 | -2.69281 |
| H | 0.77046 | 5.38876 | -3.36337 |
| H | 0.04722 | 5.90943 | -1.82728 |

**TS $^{Et}$10**

| | | | |
|---|---|---|---|
| C | -2.41298 | 3.51589 | 0.71051 |
| C | -2.19594 | 2.32783 | 1.43360 |
| C | -0.99647 | 1.61266 | 1.31500 |
| C | -0.02464 | 2.12750 | 0.45399 |
| C | -0.24074 | 3.32077 | -0.26858 |
| C | -1.43753 | 4.03310 | -0.15209 |
| N | 0.91906 | 3.53557 | -1.01979 |
| N | 1.25668 | 1.69237 | 0.09109 |
| C | 1.86100 | 2.55862 | -0.80097 |
| C | 3.19266 | 2.47070 | -2.43286 |
| C | 4.61491 | 2.60662 | -1.80777 |
| N | 3.15824 | 1.23825 | -3.02468 |
| C | 4.36111 | 0.31625 | -2.76427 |
| C | 5.09502 | 1.12891 | -1.67371 |
| H | 6.18092 | 1.00782 | -1.75751 |
| H | 4.80917 | 0.74397 | -0.68844 |
| H | -3.35474 | 4.04644 | 0.82789 |
| H | -2.97242 | 1.95900 | 2.09942 |

| | | | |
|---|---|---|---|
| H | -1.60666 | 4.95271 | -0.70511 |
| H | -0.83618 | 0.69280 | 1.87077 |
| C | 3.97550 | -1.08576 | -2.26566 |
| H | 3.35178 | -1.04893 | -1.36939 |
| H | 4.88502 | -1.64864 | -2.01898 |
| H | 3.43968 | -1.64414 | -3.03945 |
| C | 5.19128 | 0.12515 | -4.05262 |
| H | 6.04682 | -0.52982 | -3.84788 |
| H | 5.57505 | 1.06755 | -4.44540 |
| H | 4.58405 | -0.34708 | -4.83281 |
| C | 5.48029 | 3.38774 | -2.85999 |
| H | 5.46676 | 2.85694 | -3.81357 |
| H | 4.97384 | 4.34499 | -3.04108 |
| C | 4.67584 | 3.41791 | -0.47631 |
| H | 4.81536 | 4.47833 | -0.72697 |
| H | 3.69266 | 3.34742 | -0.00054 |
| C | 1.13037 | 4.68034 | -1.91355 |
| H | 1.86684 | 4.31430 | -2.64378 |
| H | 0.17834 | 4.89179 | -2.41647 |
| C | 1.95782 | 0.59480 | 0.76020 |
| H | 1.27677 | -0.26327 | 0.82198 |
| H | 2.78886 | 0.31198 | 0.11351 |
| C | 2.23266 | 0.91017 | -4.09490 |
| C | 2.38030 | 1.50783 | -5.37860 |
| C | 1.19884 | -0.04270 | -3.89167 |
| C | 1.58455 | 1.05297 | -6.43994 |
| C | 0.44026 | -0.47831 | -4.99063 |
| C | 0.64287 | 0.04087 | -6.26560 |
| H | 1.70849 | 1.50297 | -7.42243 |
| H | -0.34266 | -1.21685 | -4.83441 |
| H | 0.05099 | -0.31403 | -7.10701 |
| C | 3.31830 | 2.67669 | -5.64479 |
| H | 3.90071 | 2.83586 | -4.74246 |
| C | 2.50597 | 3.97326 | -5.86754 |
| C | 4.28973 | 2.42893 | -6.81763 |
| H | 4.85741 | 1.50226 | -6.68008 |
| H | 3.76064 | 2.35725 | -7.77611 |
| H | 5.00383 | 3.25890 | -6.89757 |
| H | 1.88997 | 3.90806 | -6.77374 |
| H | 3.18059 | 4.83276 | -5.97585 |
| H | 1.84512 | 4.15958 | -5.01492 |
| C | 0.74986 | -0.49082 | -2.50462 |
| H | 1.48911 | -0.13052 | -1.79033 |
| C | 0.61189 | -2.01905 | -2.34282 |
| C | -0.59762 | 0.19467 | -2.17394 |
| H | -0.51884 | 1.28212 | -2.26443 |
| H | -1.38036 | -0.14316 | -2.86397 |
| H | -0.92038 | -0.04254 | -1.15393 |
| H | -0.18450 | -2.41794 | -2.98255 |
| H | 0.35043 | -2.26812 | -1.30603 |
| H | 1.53768 | -2.54463 | -2.59529 |
| C | 5.73815 | 3.00061 | 0.55705 |
| H | 5.74410 | 3.71027 | 1.39482 |
| H | 5.51678 | 2.01216 | 0.97715 |
| H | 6.75354 | 2.96531 | 0.14668 |
| C | 6.95215 | 3.65003 | -2.49716 |
| H | 7.49268 | 2.72190 | -2.27225 |
| H | 7.46366 | 4.12706 | -3.34299 |
| H | 7.05576 | 4.31676 | -1.63456 |
| C | 2.47161 | 0.98360 | 2.15305 |
| H | 1.65128 | 1.30514 | 2.80404 |
| H | 2.96773 | 0.12597 | 2.62325 |
| H | 3.19472 | 1.80231 | 2.07923 |
| C | 1.64756 | 5.91543 | -1.16907 |
| H | 2.62174 | 5.70509 | -0.71460 |
| H | 1.76981 | 6.74991 | -1.87069 |
| H | 0.95864 | 6.23344 | -0.37637 |

**$^{Me}$11**

| | | | |
|---|---|---|---|
| C | -3.15894 | 0.18580 | 1.09457 |
| C | -3.08012 | 1.67166 | 0.63595 |
| N | -4.61901 | -0.01524 | 1.32197 |
| H | -2.61330 | -0.00345 | 2.02470 |
| H | -2.80753 | -0.51566 | 0.33069 |
| N | -4.50792 | 2.10171 | 0.65420 |
| H | -2.67552 | 1.78560 | -0.37499 |
| H | -2.50014 | 2.29924 | 1.32065 |
| C | -5.27697 | 1.09976 | 1.04856 |
| C | -5.18376 | -1.29056 | 1.76861 |
| H | -6.26737 | -1.19313 | 1.86963 |
| H | -4.75336 | -1.56742 | 2.73756 |
| H | -4.95686 | -2.07439 | 1.03701 |
| C | -4.93318 | 3.45503 | 0.29012 |
| H | -6.01972 | 3.53080 | 0.37735 |
| H | -4.63686 | 3.67166 | -0.74239 |
| H | -4.46406 | 4.18488 | 0.95967 |
| H | -6.35565 | 1.18526 | 1.14019 |

**$^{Et}$11**

| | | | |
|---|---|---|---|
| C | -3.07689 | 0.10361 | 0.99041 |
| C | -2.93519 | 1.60433 | 0.59859 |
| N | -4.52179 | -0.01545 | 1.34129 |
| H | -2.46644 | -0.17065 | 1.85687 |
| H | -2.83819 | -0.57133 | 0.16354 |
| N | -4.32600 | 2.12209 | 0.74918 |
| H | -2.60226 | 1.74583 | -0.43472 |
| H | -2.26081 | 2.15097 | 1.26390 |
| C | -5.12149 | 1.15143 | 1.16877 |
| C | -5.15265 | -1.27661 | 1.77823 |
| H | -6.15987 | -1.02531 | 2.12729 |
| H | -4.58639 | -1.64319 | 2.64388 |
| C | -4.70486 | 3.52570 | 0.49288 |
| H | -5.79896 | 3.56995 | 0.51483 |
| H | -4.38621 | 3.76971 | -0.52852 |
| C | -4.09433 | 4.50097 | 1.50543 |

| | | | |
|---|---|---|---|
| H | -4.41520 | 4.26379 | 2.52582 |
| H | -2.99961 | 4.49309 | 1.46869 |
| H | -4.42467 | 5.51800 | 1.26888 |
| C | -5.20204 | -2.33267 | 0.66851 |
| H | -4.19883 | -2.62016 | 0.33576 |
| H | -5.69300 | -3.23363 | 1.05147 |
| H | -5.77097 | -1.97196 | -0.19556 |
| H | -6.18068 | 1.30033 | 1.35618 |

**$^{Me}$12**

| | | | |
|---|---|---|---|
| C | -2.90710 | 1.93945 | -0.51536 |
| C | -3.10331 | 0.89183 | 0.41107 |
| C | -2.03231 | 0.15907 | 0.92580 |
| C | -0.75745 | 0.51671 | 0.47643 |
| C | -0.56071 | 1.55985 | -0.44920 |
| C | -1.63359 | 2.29460 | -0.96375 |
| H | -1.49072 | 3.10507 | -1.67151 |
| H | -3.77000 | 2.48467 | -0.88730 |
| H | -4.11289 | 0.65127 | 0.73198 |
| H | -2.18871 | -0.64480 | 1.63848 |
| N | 0.82077 | 1.63792 | -0.67823 |
| N | 0.51440 | 0.00711 | 0.77593 |
| C | 1.45520 | 0.69657 | 0.06959 |
| C | 2.96031 | 0.49572 | 0.21889 |
| N | 3.63300 | 1.53957 | 1.01030 |
| N | 3.63209 | 0.50892 | -1.08535 |
| H | 3.09058 | -0.47858 | 0.72631 |
| C | 4.92290 | 1.20860 | -0.89228 |
| C | 4.55266 | 2.27872 | 0.13078 |
| H | 5.27401 | 1.61807 | -1.84500 |
| H | 5.69808 | 0.53524 | -0.48762 |
| H | 4.08223 | 3.15366 | -0.35260 |
| H | 5.41440 | 2.63185 | 0.70772 |
| C | 1.43300 | 2.62155 | -1.58891 |
| H | 0.78303 | 2.73228 | -2.46027 |
| H | 2.40667 | 2.24129 | -1.89534 |
| H | 1.53155 | 3.58602 | -1.08145 |
| C | 0.71537 | -1.08998 | 1.73617 |
| H | 0.36182 | -0.77471 | 2.72290 |
| H | 1.76989 | -1.35090 | 1.79923 |
| H | 0.14560 | -1.96377 | 1.40630 |
| C | 3.71299 | -0.80005 | -1.73888 |
| H | 2.70600 | -1.20460 | -1.89497 |
| H | 4.30117 | -1.52977 | -1.15228 |
| H | 4.18229 | -0.68331 | -2.72036 |
| C | 2.87066 | 2.30379 | 1.98975 |
| H | 2.33411 | 1.62807 | 2.66598 |
| H | 2.14003 | 3.00649 | 1.54397 |
| H | 3.56820 | 2.88856 | 2.59779 |

**TS $^{Me}$12**

| | | | |
|---|---|---|---|
| C | -3.08088 | 1.72060 | -0.95495 |
| C | -3.31301 | 0.83073 | 0.11430 |
| C | -2.25966 | 0.28362 | 0.85301 |
| C | -0.96682 | 0.65895 | 0.47770 |
| C | -0.73455 | 1.54547 | -0.59089 |
| C | -1.78685 | 2.09703 | -1.32699 |
| H | -1.61592 | 2.78771 | -2.14746 |
| H | -3.92852 | 2.12532 | -1.50103 |
| H | -4.33494 | 0.56608 | 0.37137 |
| H | -2.44496 | -0.39833 | 1.67774 |
| N | 0.66176 | 1.69175 | -0.67639 |
| N | 0.30205 | 0.32325 | 0.98226 |
| C | 1.28738 | 0.96088 | 0.28730 |
| C | 3.33747 | 0.37359 | 0.31049 |
| N | 4.05510 | 1.23680 | 1.10907 |
| N | 3.80746 | 0.43978 | -0.97453 |
| H | 3.04823 | -0.59128 | 0.71481 |
| C | 4.87955 | 1.45527 | -1.06984 |
| C | 4.67356 | 2.25364 | 0.22888 |
| H | 4.77562 | 2.06627 | -1.97338 |
| H | 5.86294 | 0.96174 | -1.09219 |
| H | 3.98918 | 3.10589 | 0.08000 |
| H | 5.60509 | 2.62316 | 0.66468 |
| C | 1.31813 | 2.56690 | -1.65089 |
| H | 0.89216 | 2.39083 | -2.64355 |
| H | 2.38046 | 2.33479 | -1.67273 |
| H | 1.17068 | 3.61800 | -1.37916 |
| C | 0.49426 | -0.56786 | 2.12896 |
| H | 0.02227 | -0.13942 | 3.01974 |
| H | 1.55911 | -0.69202 | 2.32218 |
| H | 0.04738 | -1.54619 | 1.92261 |
| C | 3.74759 | -0.68418 | -1.90355 |
| H | 2.83945 | -1.26479 | -1.71461 |
| H | 4.62273 | -1.34480 | -1.80496 |
| H | 3.70608 | -0.31074 | -2.93235 |
| C | 3.55158 | 1.65213 | 2.41165 |
| H | 3.30366 | 0.77400 | 3.01522 |
| H | 2.65139 | 2.28216 | 2.30889 |
| H | 4.32998 | 2.21534 | 2.93333 |

**$^{Et}$12**

| | | | |
|---|---|---|---|
| C | -3.00418 | 2.10637 | -0.33921 |
| C | -3.19367 | 1.03022 | 0.55579 |
| C | -2.12097 | 0.27143 | 1.02554 |
| C | -0.84898 | 0.62901 | 0.56572 |
| C | -0.65981 | 1.69929 | -0.33240 |
| C | -1.73601 | 2.46113 | -0.80070 |
| H | -1.59877 | 3.28890 | -1.48901 |
| H | -3.86816 | 2.67155 | -0.67738 |
| H | -4.19953 | 0.78769 | 0.88685 |
| H | -2.27515 | -0.55501 | 1.71237 |
| N | 0.71923 | 1.78093 | -0.57757 |

| | | | |
|---|---|---|---|
| N | 0.42522 | 0.10836 | 0.83400 |
| C | 1.35404 | 0.80791 | 0.12499 |
| C | 2.84976 | 0.55727 | 0.22092 |
| N | 3.59431 | 1.55381 | 1.01858 |
| N | 3.47566 | 0.56712 | -1.10863 |
| H | 2.95791 | -0.43408 | 0.70239 |
| C | 4.83490 | 1.11749 | -0.91003 |
| C | 4.59570 | 2.19116 | 0.14713 |
| H | 5.22536 | 1.52315 | -1.84698 |
| H | 5.53750 | 0.35178 | -0.53463 |
| H | 4.22954 | 3.13056 | -0.30825 |
| H | 5.50273 | 2.42536 | 0.71287 |
| C | 1.31692 | 2.76511 | -1.51291 |
| H | 2.37603 | 2.83654 | -1.27943 |
| H | 0.84507 | 3.72794 | -1.28935 |
| C | 0.66623 | -1.05411 | 1.72253 |
| H | -0.09621 | -1.00218 | 2.50543 |
| H | 1.63434 | -0.91498 | 2.20883 |
| C | 3.40123 | -0.73650 | -1.79215 |
| H | 2.34170 | -1.02699 | -1.82898 |
| H | 3.92835 | -1.51248 | -1.20142 |
| C | 2.86422 | 2.41401 | 1.95708 |
| H | 2.12863 | 1.79167 | 2.48280 |
| H | 2.29656 | 3.20735 | 1.42927 |
| C | 3.96626 | -0.69151 | -3.21292 |
| H | 5.04268 | -0.48969 | -3.21445 |
| H | 3.81146 | -1.65727 | -3.70596 |
| H | 3.47140 | 0.08252 | -3.81060 |
| C | 3.79733 | 3.05934 | 2.98665 |
| H | 3.21164 | 3.63407 | 3.71273 |
| H | 4.36805 | 2.29386 | 3.52391 |
| H | 4.50462 | 3.74949 | 2.51400 |
| C | 0.59830 | -2.38454 | 0.96722 |
| H | 1.38946 | -2.44971 | 0.21252 |
| H | 0.72798 | -3.21308 | 1.67175 |
| H | -0.36895 | -2.50637 | 0.46827 |
| C | 1.11155 | 2.36065 | -2.97439 |
| H | 1.53513 | 3.13256 | -3.62611 |
| H | 1.62382 | 1.41663 | -3.17927 |
| H | 0.05080 | 2.25070 | -3.22145 |

**TS $^{Et}$12**

| | | | |
|---|---|---|---|
| C | -3.12608 | 1.43539 | -1.14295 |
| C | -3.34037 | 0.54669 | -0.06869 |
| C | -2.28410 | 0.09082 | 0.72448 |
| C | -1.00459 | 0.55393 | 0.40171 |
| C | -0.79018 | 1.43828 | -0.67326 |
| C | -1.84749 | 1.89854 | -1.46431 |
| H | -1.69086 | 2.58436 | -2.29161 |
| H | -3.97528 | 1.76849 | -1.73322 |
| H | -4.35057 | 0.21068 | 0.14836 |
| H | -2.45791 | -0.59172 | 1.55097 |
| N | 0.59570 | 1.67524 | -0.71046 |
| N | 0.26399 | 0.30908 | 0.95885 |
| C | 1.22891 | 1.00487 | 0.29102 |
| C | 3.26561 | 0.43791 | 0.29279 |
| N | 4.01572 | 1.32032 | 1.04395 |
| N | 3.69724 | 0.45625 | -1.00567 |
| H | 2.99096 | -0.51267 | 0.74008 |
| C | 4.76497 | 1.46426 | -1.17247 |
| C | 4.60838 | 2.30430 | 0.10744 |
| H | 4.62622 | 2.04851 | -2.08927 |
| H | 5.74977 | 0.97774 | -1.21399 |
| H | 3.92298 | 3.15511 | -0.04434 |
| H | 5.55885 | 2.68271 | 0.48728 |
| C | 1.23694 | 2.61608 | -1.64520 |
| H | 0.74061 | 2.50175 | -2.61512 |
| H | 2.27061 | 2.29090 | -1.76596 |
| C | 0.47286 | -0.49908 | 2.17377 |
| H | 1.52545 | -0.79129 | 2.20299 |
| H | -0.11621 | -1.41702 | 2.06548 |
| C | 3.52701 | -0.67767 | -1.92050 |
| H | 2.52618 | -1.09123 | -1.74257 |
| H | 3.52454 | -0.27938 | -2.94282 |
| C | 3.52098 | 1.77499 | 2.34710 |
| H | 3.15249 | 0.89049 | 2.87891 |
| H | 2.65376 | 2.44324 | 2.19024 |
| C | 0.08464 | 0.25512 | 3.45103 |
| H | -0.97072 | 0.54541 | 3.43427 |
| H | 0.24884 | -0.38463 | 4.32514 |
| H | 0.68695 | 1.16237 | 3.56615 |
| C | 1.15574 | 4.06590 | -1.15485 |
| H | 1.63346 | 4.73440 | -1.87979 |
| H | 0.11541 | 4.38482 | -1.03056 |
| H | 1.66484 | 4.17949 | -0.19112 |
| C | 4.59818 | -1.76962 | -1.77215 |
| H | 4.59941 | -2.18654 | -0.75798 |
| H | 4.40141 | -2.58660 | -2.47555 |
| H | 5.60001 | -1.38031 | -1.98463 |
| C | 4.59957 | 2.46800 | 3.18127 |
| H | 4.19442 | 2.72258 | 4.16638 |
| H | 5.46627 | 1.81319 | 3.32410 |
| H | 4.93929 | 3.39984 | 2.71615 |

**$^{Me}$13**

| | | | |
|---|---|---|---|
| C | -0.61820 | -1.54180 | -0.24707 |
| C | 0.29617 | -2.58247 | -0.42460 |
| C | -0.20456 | -0.28745 | 0.25120 |
| C | 1.14293 | -0.12137 | 0.55894 |
| C | 2.05891 | -1.18891 | 0.42366 |
| C | 1.65773 | -2.41925 | -0.08951 |
| N | 1.84604 | 1.00275 | 1.02576 |
| N | 3.31474 | -0.74876 | 0.87652 |
| C | 3.20379 | 0.62478 | 1.24378 |

| | | | |
|---|---|---|---|
| C | 4.20317 | 1.42277 | 1.71296 |
| N | 4.13474 | 2.86281 | 1.76025 |
| N | 5.45962 | 0.93128 | 2.22323 |
| C | 6.31847 | 2.13235 | 2.35952 |
| C | 5.30193 | 3.27929 | 2.57450 |
| H | 6.88665 | 2.28670 | 1.43175 |
| H | 7.02634 | 2.00850 | 3.18427 |
| H | 5.66639 | 4.25924 | 2.25282 |
| H | 5.00952 | 3.34520 | 3.63164 |
| C | 4.06073 | 3.51049 | 0.43334 |
| H | 4.95373 | 3.32257 | -0.19057 |
| H | 3.93677 | 4.59157 | 0.56602 |
| H | 3.18744 | 3.12730 | -0.10332 |
| C | 5.34037 | 0.12938 | 3.45949 |
| H | 4.67258 | -0.71736 | 3.27345 |
| H | 4.93253 | 0.70444 | 4.31095 |
| H | 6.32712 | -0.26312 | 3.73146 |
| C | 4.54467 | -1.31182 | 0.32229 |
| H | 5.40321 | -0.91917 | 0.87105 |
| H | 4.65637 | -1.04990 | -0.74256 |
| H | 4.51664 | -2.40180 | 0.41692 |
| C | 1.17598 | 2.01270 | 1.84306 |
| H | 1.85654 | 2.84871 | 2.01724 |
| H | 0.87124 | 1.59655 | 2.81720 |
| H | 0.28497 | 2.36909 | 1.31686 |
| H | -0.91792 | 0.52271 | 0.37553 |
| H | -1.66510 | -1.69350 | -0.49870 |
| H | -0.04134 | -3.53630 | -0.82288 |
| H | 2.36245 | -3.23631 | -0.21791 |

**TS $^{Me}$13**

| | | | |
|---|---|---|---|
| C | -0.24787 | -2.10962 | 0.48315 |
| C | 0.86487 | -2.91734 | 0.19857 |
| C | -0.11894 | -0.72146 | 0.65756 |
| C | 1.15803 | -0.16702 | 0.53999 |
| C | 2.28041 | -0.98563 | 0.25917 |
| C | 2.15172 | -2.36403 | 0.08331 |
| N | 1.63884 | 1.14171 | 0.60480 |
| N | 3.37444 | -0.12357 | 0.18803 |
| C | 3.03055 | 1.19686 | 0.47813 |
| C | 3.87166 | 1.82621 | 2.18387 |
| N | 4.53404 | 3.02890 | 2.04168 |
| N | 4.82111 | 0.91903 | 2.59131 |
| C | 6.16453 | 1.51563 | 2.74366 |
| C | 5.99938 | 2.80941 | 1.93933 |
| H | 6.95218 | 0.85903 | 2.35074 |
| H | 6.38019 | 1.71828 | 3.80734 |
| H | 6.28723 | 2.66107 | 0.88106 |
| H | 6.56394 | 3.65668 | 2.34300 |
| C | 3.95719 | 4.08636 | 1.23340 |
| H | 3.86283 | 3.76273 | 0.18009 |
| H | 4.58620 | 4.98117 | 1.29494 |
| H | 2.96050 | 4.33589 | 1.60756 |
| C | 4.47348 | -0.28301 | 3.32633 |
| H | 3.45579 | -0.57878 | 3.06050 |
| H | 4.51755 | -0.12298 | 4.41815 |
| H | 5.16014 | -1.10357 | 3.07506 |
| C | 4.72034 | -0.54035 | -0.15999 |
| H | 5.32110 | 0.35669 | -0.32276 |
| H | 4.70549 | -1.13749 | -1.08112 |
| H | 5.17733 | -1.13819 | 0.63981 |
| C | 0.89557 | 2.27313 | 1.12310 |
| H | 1.29778 | 2.52859 | 2.11763 |
| H | -0.16405 | 2.01960 | 1.20368 |
| H | 1.00561 | 3.13816 | 0.46160 |
| H | -0.98883 | -0.10644 | 0.87254 |
| H | -1.23132 | -2.56564 | 0.57003 |
| H | 0.73036 | -3.98812 | 0.06526 |
| H | 3.01399 | -2.98998 | -0.13197 |

**$^{Et}$13**

| | | | |
|---|---|---|---|
| C | -0.67055 | -1.57136 | -0.33749 |
| C | 0.25113 | -2.59051 | -0.58112 |
| C | -0.26054 | -0.34115 | 0.22235 |
| C | 1.08760 | -0.18086 | 0.53040 |
| C | 2.01258 | -1.23289 | 0.33381 |
| C | 1.61392 | -2.43704 | -0.24415 |
| N | 1.77904 | 0.91936 | 1.06584 |
| N | 3.26745 | -0.80131 | 0.79019 |
| C | 3.15218 | 0.55443 | 1.21969 |
| C | 4.14351 | 1.37621 | 1.66608 |
| N | 4.03965 | 2.80988 | 1.65854 |
| N | 5.42022 | 0.93585 | 2.18431 |
| C | 6.22702 | 2.17124 | 2.36448 |
| C | 5.16583 | 3.29326 | 2.48340 |
| H | 6.87347 | 2.32975 | 1.49299 |
| H | 6.86269 | 2.08698 | 3.25055 |
| H | 5.51806 | 4.26686 | 2.12955 |
| H | 4.83942 | 3.40290 | 3.52769 |
| C | 3.91695 | 3.42161 | 0.31082 |
| H | 3.75029 | 4.49688 | 0.45817 |
| H | 3.00402 | 3.01688 | -0.13857 |
| C | 5.32985 | 0.09580 | 3.40546 |
| H | 4.51161 | -0.61270 | 3.24553 |
| H | 5.04936 | 0.70708 | 4.28540 |
| C | 4.51381 | -1.37505 | 0.26420 |
| H | 5.29956 | -0.63136 | 0.41416 |
| H | 4.39164 | -1.53367 | -0.81856 |
| C | 1.10684 | 1.83025 | 2.01179 |
| H | 1.86688 | 2.18829 | 2.70970 |
| H | 0.36954 | 1.23987 | 2.57690 |
| H | -0.97682 | 0.45862 | 0.38582 |
| H | -1.71828 | -1.71722 | -0.58906 |
| H | -0.08054 | -3.52338 | -1.03086 |

| | | | |
|---|---|---|---|
| H | 2.31779 | -3.24478 | -0.41815 |
| C | 0.41419 | 3.02128 | 1.33832 |
| H | 1.14156 | 3.66871 | 0.84025 |
| H | -0.31808 | 2.69193 | 0.59300 |
| H | -0.11493 | 3.61766 | 2.09278 |
| C | 4.90677 | -2.69292 | 0.94731 |
| H | 4.14252 | -3.46508 | 0.81326 |
| H | 5.84611 | -3.06828 | 0.52181 |
| H | 5.05107 | -2.54712 | 2.02229 |
| C | 6.62870 | -0.66547 | 3.68500 |
| H | 6.50539 | -1.31761 | 4.55889 |
| H | 6.90745 | -1.28391 | 2.82442 |
| H | 7.46373 | 0.01373 | 3.89392 |
| C | 5.09564 | 3.18990 | -0.65272 |
| H | 6.01601 | 3.66941 | -0.29774 |
| H | 5.28762 | 2.11728 | -0.77237 |
| H | 4.86324 | 3.60600 | -1.64149 |

**TS $^{Et}$13**

| | | | |
|---|---|---|---|
| C | -0.22807 | -2.48463 | 0.97608 |
| C | 0.89509 | -3.24619 | 0.61622 |
| C | -0.14481 | -1.09129 | 1.13825 |
| C | 1.09799 | -0.48689 | 0.93094 |
| C | 2.23120 | -1.25692 | 0.57165 |
| C | 2.14677 | -2.64046 | 0.40828 |
| N | 1.52444 | 0.83938 | 0.96914 |
| N | 3.28015 | -0.34603 | 0.42633 |
| C | 2.89271 | 0.96355 | 0.70699 |
| C | 3.86614 | 1.75893 | 2.24640 |
| N | 4.47125 | 2.97464 | 1.95786 |
| N | 4.88283 | 0.91396 | 2.61638 |
| C | 6.21729 | 1.54530 | 2.56868 |
| C | 5.92368 | 2.77498 | 1.70333 |
| H | 6.97098 | 0.87713 | 2.12922 |
| H | 6.55794 | 1.83363 | 3.57634 |
| H | 6.09277 | 2.56148 | 0.62989 |
| H | 6.51496 | 3.65083 | 1.98397 |
| C | 3.76968 | 3.94541 | 1.12915 |
| H | 3.71973 | 3.56867 | 0.08894 |
| H | 2.74056 | 3.99380 | 1.49543 |
| C | 4.64285 | -0.29643 | 3.39157 |
| H | 3.68442 | -0.70903 | 3.06070 |
| H | 5.42053 | -1.03272 | 3.13862 |
| C | 4.59360 | -0.68958 | -0.10998 |
| H | 5.27896 | 0.10098 | 0.20273 |
| H | 4.92957 | -1.62363 | 0.36015 |
| C | 0.73639 | 1.95272 | 1.47739 |
| H | -0.11581 | 1.54018 | 2.02967 |
| H | 1.37843 | 2.47272 | 2.20459 |
| H | -1.02201 | -0.50852 | 1.40679 |
| H | -1.18435 | -2.98017 | 1.12659 |
| H | 0.79581 | -4.32164 | 0.48963 |
| H | 3.01384 | -3.23272 | 0.12753 |
| C | 0.25176 | 2.89858 | 0.37183 |
| H | 1.10074 | 3.27698 | -0.20658 |
| H | -0.42702 | 2.38041 | -0.31638 |
| H | -0.28285 | 3.75324 | 0.80574 |
| C | 4.58275 | -0.82337 | -1.63968 |
| H | 5.58233 | -1.08450 | -2.00925 |
| H | 3.88232 | -1.60172 | -1.96333 |
| H | 4.27792 | 0.12517 | -2.09599 |
| C | 4.61150 | -0.05956 | 4.91197 |
| H | 3.82600 | 0.66350 | 5.15968 |
| H | 4.40466 | -0.99730 | 5.44319 |
| H | 5.56875 | 0.33047 | 5.27921 |
| C | 4.39428 | 5.34378 | 1.17569 |
| H | 4.46069 | 5.70968 | 2.20787 |
| H | 5.40061 | 5.36089 | 0.74044 |
| H | 3.77717 | 6.04483 | 0.60101 |

**$^{Me}$14**

| | | | |
|---|---|---|---|
| C | -4.08519 | 9.39480 | -0.03172 |
| C | -3.37679 | 8.01492 | 0.07536 |
| C | -5.55065 | 9.21503 | 0.48329 |
| H | -4.06323 | 9.76693 | -1.05891 |
| H | -3.56469 | 10.12373 | 0.59704 |
| N | -4.35645 | 7.26524 | 1.02938 |
| C | -5.46133 | 7.90611 | 1.19466 |
| C | -5.98209 | 10.33412 | 1.46216 |
| H | -5.29597 | 10.40824 | 2.31313 |
| H | -6.99519 | 10.16204 | 1.84258 |
| H | -5.97692 | 11.29413 | 0.93429 |
| C | -6.59223 | 9.08676 | -0.66570 |
| H | -6.31266 | 8.31040 | -1.38476 |
| H | -6.64912 | 10.04355 | -1.19599 |
| H | -7.58881 | 8.85509 | -0.27396 |
| C | -3.31408 | 7.25884 | -1.26053 |
| H | -4.28455 | 7.21587 | -1.76102 |
| H | -2.93866 | 6.24087 | -1.12361 |
| H | -2.61739 | 7.78912 | -1.91793 |
| C | -1.97742 | 8.09521 | 0.69031 |
| H | -1.96658 | 8.66998 | 1.61862 |
| H | -1.32045 | 8.60008 | -0.02584 |
| H | -1.56577 | 7.09908 | 0.87992 |
| H | -6.25049 | 7.47464 | 1.80875 |
| C | -4.07175 | 5.95927 | 1.62371 |
| C | -4.49524 | 4.79609 | 0.94322 |
| C | -3.40102 | 5.93296 | 2.86701 |
| C | -4.12760 | 3.56545 | 1.50904 |
| C | -3.06672 | 4.67140 | 3.37971 |
| C | -3.40230 | 3.50169 | 2.69787 |
| H | -4.43028 | 2.64533 | 1.01765 |
| H | -2.55149 | 4.60532 | 4.33348 |
| H | -3.12395 | 2.53539 | 3.11103 |

| | | | |
|---|---|---|---|
| C | -5.41718 | 4.81871 | -0.27410 |
| H | -5.46407 | 5.84008 | -0.66123 |
| C | -6.85526 | 4.43471 | 0.15426 |
| C | -4.92403 | 3.91628 | -1.42419 |
| H | -3.89885 | 4.16271 | -1.72142 |
| H | -4.94550 | 2.85802 | -1.14247 |
| H | -5.57261 | 4.03546 | -2.29940 |
| H | -6.88870 | 3.40944 | 0.53957 |
| H | -7.53773 | 4.49909 | -0.70111 |
| H | -7.23061 | 5.09639 | 0.94494 |
| C | -3.15982 | 7.18365 | 3.71011 |
| H | -3.30144 | 8.06560 | 3.07771 |
| C | -1.73320 | 7.25966 | 4.29114 |
| C | -4.22376 | 7.26409 | 4.83291 |
| H | -5.24210 | 7.25877 | 4.42418 |
| H | -4.13754 | 6.40999 | 5.51410 |
| H | -4.09275 | 8.18167 | 5.41812 |
| H | -1.55286 | 6.46322 | 5.02112 |
| H | -1.58936 | 8.21492 | 4.80854 |
| H | -0.97266 | 7.17512 | 3.50736 |

**$^{Et}$14**

| | | | |
|---|---|---|---|
| C | -7.21227 | 8.44782 | 0.67900 |
| C | -7.26284 | 6.90559 | 0.48630 |
| C | -5.85319 | 8.95754 | 0.09598 |
| H | -7.26556 | 8.68734 | 1.74555 |
| H | -8.06505 | 8.92622 | 0.19278 |
| N | -5.77078 | 6.60924 | 0.16054 |
| C | -5.09242 | 7.68565 | -0.04586 |
| C | -5.99845 | 9.58881 | -1.33402 |
| H | -6.53600 | 8.87471 | -1.97065 |
| H | -5.00163 | 9.70439 | -1.77703 |
| C | -5.12420 | 9.91125 | 1.09579 |
| H | -5.01513 | 9.37827 | 2.05015 |
| H | -5.80807 | 10.74553 | 1.29381 |
| C | -7.70120 | 6.14949 | 1.74379 |
| H | -7.14628 | 6.46538 | 2.62962 |
| H | -7.59226 | 5.06764 | 1.61915 |
| H | -8.76116 | 6.36359 | 1.91687 |
| C | -8.12922 | 6.47318 | -0.70648 |
| H | -7.88401 | 7.02319 | -1.61849 |
| H | -9.17555 | 6.67902 | -0.45811 |
| H | -8.03416 | 5.40101 | -0.90018 |
| H | -4.04126 | 7.61124 | -0.31594 |
| C | -5.20808 | 5.26238 | 0.07267 |
| C | -4.68726 | 4.68864 | 1.25422 |
| C | -5.18846 | 4.61285 | -1.18104 |
| C | -4.22379 | 3.36812 | 1.16651 |
| C | -4.71292 | 3.29249 | -1.20080 |
| C | -4.25934 | 2.66821 | -0.03970 |
| H | -3.81528 | 2.88844 | 2.05113 |
| H | -4.68232 | 2.75447 | -2.14385 |
| H | -3.90296 | 1.64192 | -0.08069 |
| C | -4.49172 | 5.47952 | 2.54645 |
| H | -5.08765 | 6.39558 | 2.49069 |
| C | -3.01102 | 5.91778 | 2.66608 |
| C | -4.94766 | 4.71289 | 3.80444 |
| H | -5.98612 | 4.37538 | 3.71663 |
| H | -4.32269 | 3.83248 | 3.98884 |
| H | -4.86934 | 5.35888 | 4.68623 |
| H | -2.34983 | 5.04630 | 2.73201 |
| H | -2.86415 | 6.52658 | 3.56579 |
| H | -2.69413 | 6.50712 | 1.79629 |
| C | -5.52778 | 5.31173 | -2.49568 |
| H | -6.02365 | 6.25972 | -2.27141 |
| C | -6.48432 | 4.49399 | -3.38787 |
| C | -4.22183 | 5.65791 | -3.25303 |
| H | -3.55294 | 6.27507 | -2.64022 |
| H | -3.67401 | 4.74891 | -3.52592 |
| H | -4.44947 | 6.20751 | -4.17378 |
| H | -6.01524 | 3.56817 | -3.73814 |
| H | -6.76139 | 5.07633 | -4.27390 |
| H | -7.40250 | 4.22315 | -2.85515 |
| C | -3.75923 | 10.44869 | 0.64302 |
| H | -3.03758 | 9.64508 | 0.45028 |
| H | -3.83535 | 11.05677 | -0.26426 |
| H | -3.33147 | 11.08244 | 1.42703 |
| C | -6.72837 | 10.94022 | -1.34744 |
| H | -7.72568 | 10.87174 | -0.89819 |
| H | -6.16881 | 11.71395 | -0.81245 |
| H | -6.85430 | 11.27852 | -2.38150 |

**$^{Me}$15**

| | | | |
|---|---|---|---|
| C | -3.20242 | 0.14700 | 0.99264 |
| C | -3.10171 | 1.62031 | 0.55934 |
| N | -4.66581 | 0.00889 | 1.25097 |
| H | -2.63390 | -0.06169 | 1.91184 |
| H | -2.86986 | -0.55666 | 0.21956 |
| N | -4.45759 | 2.13214 | 0.91490 |
| H | -2.92505 | 1.73153 | -0.52196 |
| H | -2.31861 | 2.17547 | 1.09031 |
| C | -5.34952 | 1.17457 | 1.25300 |
| C | -5.20472 | -1.26031 | 1.70183 |
| H | -6.28052 | -1.14176 | 1.84874 |
| H | -4.74561 | -1.57702 | 2.65293 |
| H | -5.02398 | -2.04990 | 0.95736 |
| C | -4.80082 | 3.51646 | 0.64905 |
| H | -5.83619 | 3.67670 | 0.95774 |
| H | -4.70476 | 3.75550 | -0.42299 |
| H | -4.14435 | 4.19844 | 1.20980 |

**$^{Et}$15**

| | | | |
|---|---|---|---|
| C | -3.09502 | 0.13263 | 1.05588 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C | -2.97746 | 1.58503 | 0.55958 | C | -4.68627 | 3.49755 | 0.53906 |
| N | -4.56790 | 0.00315 | 1.26601 | H | -5.77647 | 3.56438 | 0.60045 |
| H | -2.56340 | -0.03271 | 2.00573 | H | -4.39456 | 3.72527 | -0.50042 |
| H | -2.72598 | -0.59783 | 0.32776 | C | -4.03038 | 4.50551 | 1.49623 |
| N | -4.34641 | 2.11221 | 0.83972 | H | -4.33994 | 4.30739 | 2.52903 |
| H | -2.76403 | 1.64617 | -0.51884 | H | -2.93537 | 4.45636 | 1.44978 |
| H | -2.20886 | 2.15616 | 1.09147 | H | -4.32787 | 5.52844 | 1.23352 |
| C | -5.24817 | 1.16792 | 1.18803 | C | -5.15127 | -2.34587 | 0.63335 |
| C | -5.14788 | -1.25588 | 1.71707 | H | -4.13496 | -2.59110 | 0.30080 |
| H | -6.17011 | -1.02610 | 2.03180 | H | -5.60486 | -3.26663 | 1.02121 |
| H | -4.59605 | -1.61179 | 2.60362 | H | -5.72762 | -2.01437 | -0.23823 |

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