Supplementary Material for

Reversible CO_2 fixation by N-heterocyclic imines forming water-stable zwitterionic nitrogen-base–CO_2 adducts

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CONTENTS:

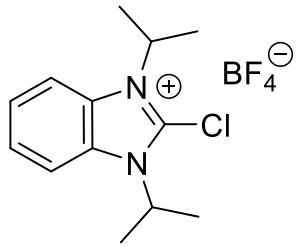
Synthetic Details

General remarks: All manipulations were performed under an inert atmosphere of dry argon, using standard Schlenk and drybox techniques. Dry and oxygen-free solvents were employed. ^{1}H, ^{13}C and ^{15}N spectra were recorded at 300 K on Bruker AVANCE I 400, Bruker AVANCE III 400 or Bruker AVANCE II 200 spectrometers. Low temperature NMR spectra were recorded on a Bruker AVANCE III 400 spectrometer at the temperatures indicated. All other spectra were obtained at 25 °C in the solvent indicated. Chemical shifts are given in parts per million (ppm) relative to $SiMe_4$ (^{1}H, ^{13}C) or NH_3 (^{15}N) and were referenced internally to the residual solvent signals. NMR multiplicities are abbreviated as follows: s = singlet, d = doublet, t = triplet, sept = septet, m = multiplet, br = broad signal. Mass spectra were obtained with an Orbitrap LTQ XL (Thermo Scientific) spectrometer. IR spectra were obtained on a Bruker ALPHA II FT-IR spectrometer. The N-heterocyclic imines **2c**,[1] **4a**,[2] **4b**,[2] **4c**,[3] **4d**[3] and **4e**[3] and the azolium salts[4–6] were prepared following literature procedures. Carbon dioxide was purchased from Westfalen AG (Münster) as carbon dioxide 4.5 (99.995%). All other compounds were purchased from commercial sources.

Preparation of 2-chloroazolium salts

The 2-chloroazolium salts were prepared according to a modified literature procedure:

Synthesis of 2-chloro-1,3-diisopropylbenzimidazolium tetrafluoroborate: A solution of sodium hexamethyldisilazane (NaHMDS) in THF (7.77 mL, 7.77 mmol, 1 M in THF, 1.10 eq.) was added dropwise to a stirred suspension of 1,3-diisopropylbenzimidazolium bromide (2.00 g, 7.06 mmol, 1.00 eq.) in THF (30 mL) at -78 °C. The cold bath was removed, and the solution was stirred at room temperature for 2 hours. The resulting solution of the free carbene was filtered into a flask containing a solution of hexachloroethane (2.24 g, 9.46 mmol, 1.34 eq.) in THF (30 mL) at -78 °C. After complete addition, the cold bath was removed and the mixture was stirred at room temperature overnight. Toluene was added until the precipitation of the benzimidazolium chloride salt was complete. The precipitate was collected on a frit and washed twice with Et_2O (2 x 20 mL). The isolated solid was dissolved in $CHCl_3$ (80 mL) and transferred to a separation funnel. An aqueous solution (80 mL) of $NaBF_4$ (3.88 g, 35.30 mmol, 5.00 eq.) was added and the two-phase mixture was shaken vigorously. The organic phase was separated, and the aqueous phase was extracted once with a small portion of $CHCl_3$. The combined $CHCl_3$ fractions were dried (anhydrous $MgSO_4$), filtered, and the volatiles were evaporated. The resulting solid was dried *in vacuo* at 80 °C for 18 hours, yielding 2-chloro-1,3-diisopropylbenzimidazolium tetrafluoroborate as a colorless solid. Yield 81% (1.86 g, 5.73 mmol).



^{1}H NMR (400.13 MHz, $CDCl_3$): δ = 7.88-7.90 (m, 2H, aryl-H), 7.57-7.60 (m, 2H, aryl-H), 5.18 (sept, $^{3}J_{HH}$ = 7.0 Hz, 2H, $CH(CH_3)_2$), 1.74 (d, $^{3}J_{HH}$ = 6.9 Hz, 12H, CH_3).

$^{13}C\{^{1}H\}$ NMR (100.62 MHz, $CDCl_3$): δ = 137.7 ($ClCN_2$), 130.2 (*ipso*-C), 127.1 (aryl-C), 114.5 (aryl-C), 53.9 ($CH(CH_3)_2$), 20.5 (CH_3).

^{11}B NMR (128.38 MHz, $CDCl_3$): δ = -1.2.

$^{11}B\{^{1}H\}$ NMR (128.38 MHz, $CDCl_3$): δ = -1.2.

^{19}F NMR (376.37 MHz, $CDCl_3$): δ = -153.5.

$^{19}F\{^{1}H\}$ NMR (376.37 MHz, $CDCl_3$): δ = -153.5.

HRMS (ESI): m/z calculated for $[C_{13}H_{18}ClN_2]^+$ $(M)^+$ 237.11530, found 237.11502.
Elemental analysis: calculated (%) for $C_{13}H_{18}BClF_4N_2$: C 48.11, H 5.59, N 8.63, found C 47.82, H 5.33, N 8.63
IR (neat): $\tilde{\nu}$ = 1034 (vs), 1046 (vs), 1094 (s), 1146 (w), 1182 (w), 1303 (m), 1379 (m), 1399 (m), 1435 (s), 1475 (s), 1512 (m), 2948 (w), 2994 (w).

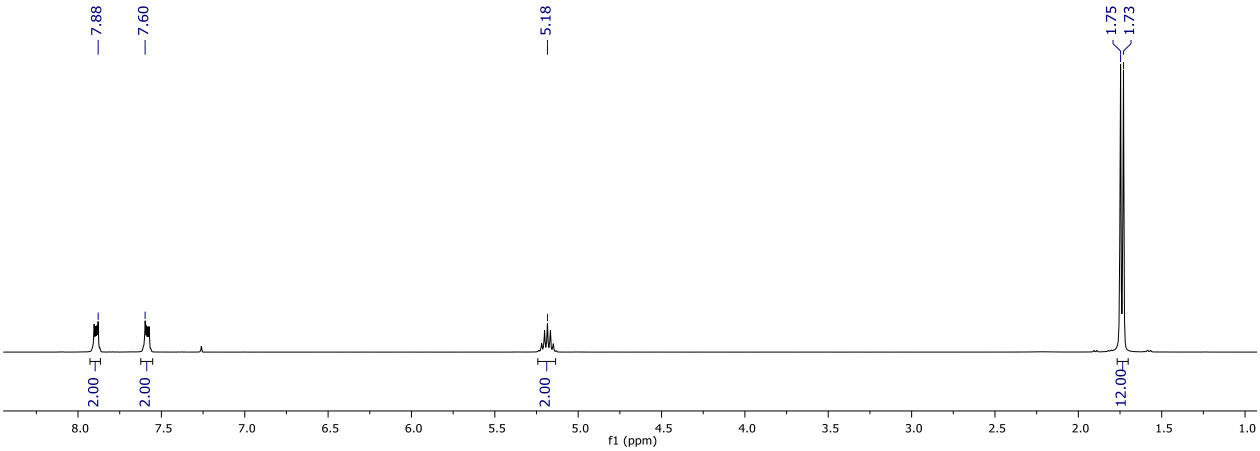


Figure S1: ^{1}H NMR spectrum (in $CDCl_3$, 300 K, 400.13 MHz) of 2-chloro-1,3-diisopropylbenzimidazolium tetrafluoroborate.

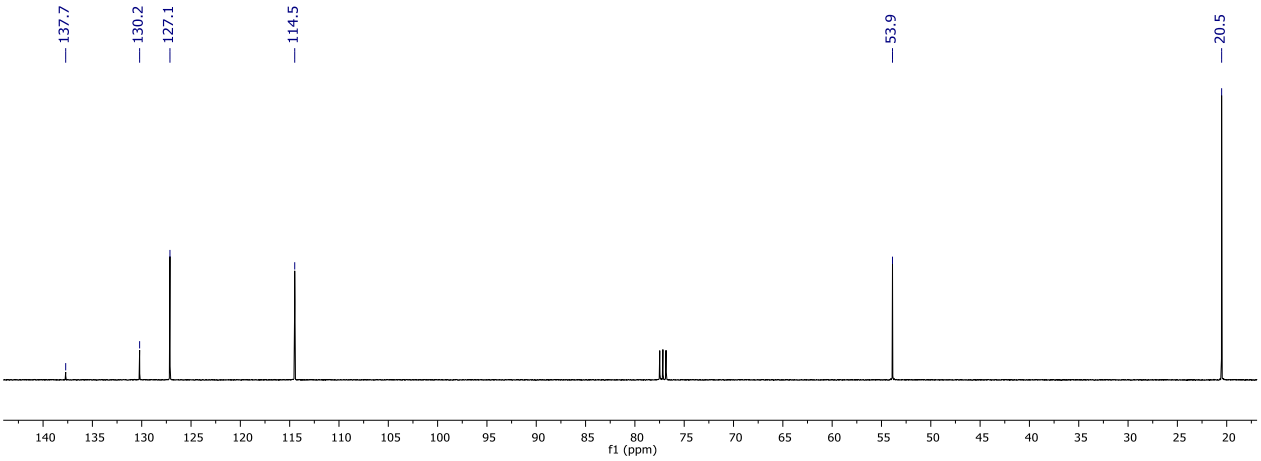


Figure S2: $^{13}C\{^{1}H\}$ NMR spectrum (in $CDCl_3$, 300 K, 100.62 MHz) of 2-chloro-1,3-diisopropylbenzimidazolium tetrafluoroborate.

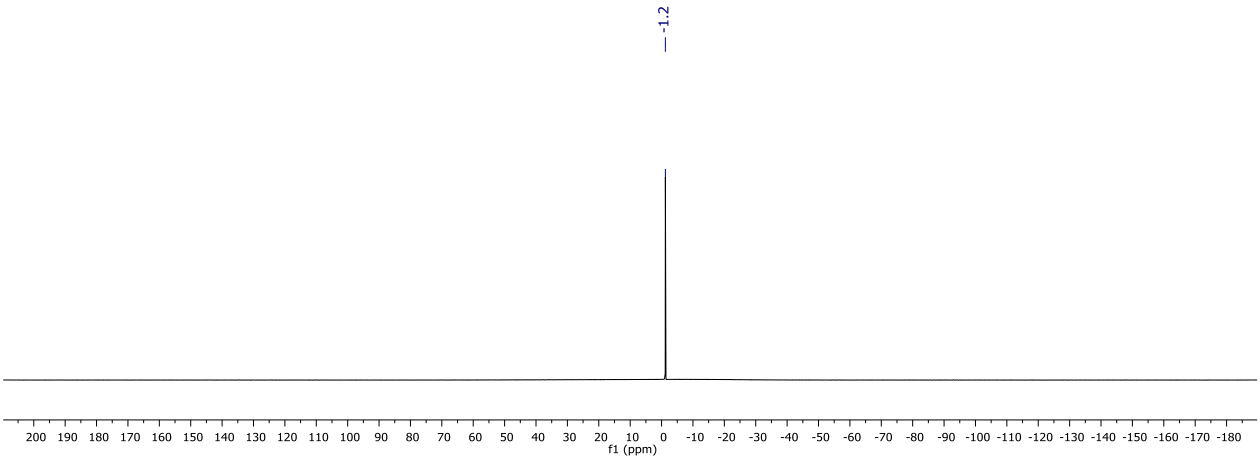


Figure S3: ^{11}B NMR spectrum (in $CDCl_3$, 300 K, 128.38 MHz) of 2-chloro-1,3-diisopropylbenzimidazolium tetrafluoroborate.

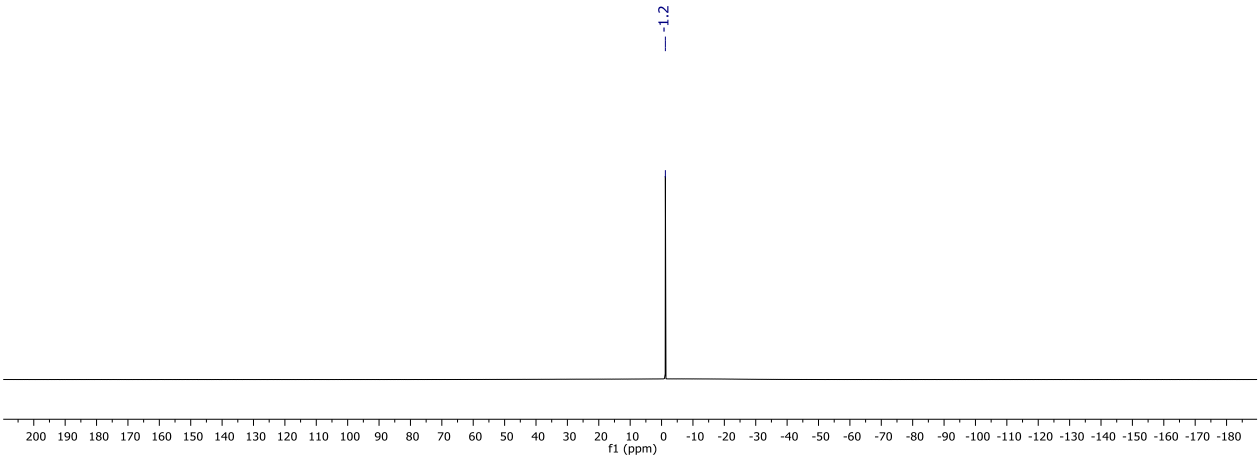


Figure S4: ^{11}B{H} NMR spectrum (in $CDCl_3$, 300 K, 128.38 MHz) of 2-chloro-1,3-diisopropylbenzimidazolium tetrafluoroborate.

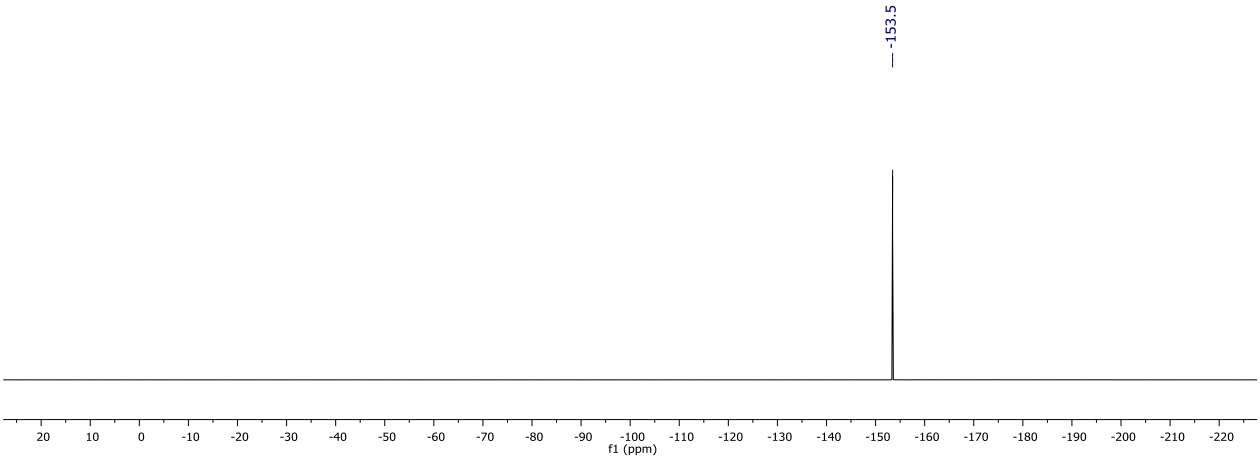


Figure S5: ^{19}F NMR spectrum (in $CDCl_3$, 300 K, 376.37 MHz) of 2-chloro-1,3-diisopropylbenzimidazolium tetrafluoroborate.

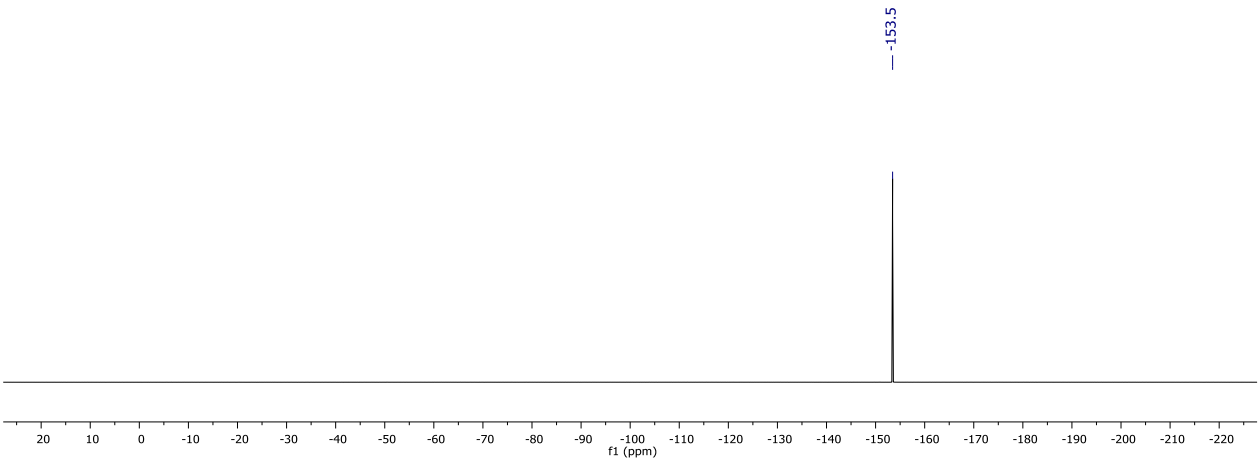
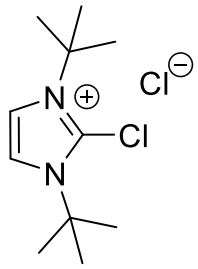


Figure S6: $^{19}F\{H\}$ NMR spectrum (in $CDCl_3$, 300 K, 376.37 MHz) of 2-chloro-1,3-diisopropylbenzimidazolium tetrafluoroborate.

Synthesis of 2-chloro-1,3-di-*tert*-butylimidazolium chloride: A Schlenk flask containing 1,3-di-*tert*-butylimidazolium tetrafluoroborate (10.00 g, 37.30 mmol, 1.00 eq.) and KO*t*Bu (4.19 g, 37.30 mmol, 1.00 eq.) was cooled to -78 °C. After slowly adding THF (100 mL), the cold bath was removed, and the solution was stirred at room temperature for 2 hours. The volatiles were removed under reduced pressure to afford a colorless solid. The free carbene was extracted with *n*-hexane and the insoluble KBF_4 was filtered off. The *n*-hexane was evaporated and the resulting solid was dissolved in THF (80 mL). Hexachloroethane (11.83 g, 49.98 mmol, 1.34 eq.) was added and the reaction mixture was stirred at room temperature overnight. Toluene was added until the precipitation of the imidazolium chloride salt was complete. The precipitate was collected on a frit and washed twice with Et_2O (2 x 40 mL). The volatiles were evaporated and the solid product was dried in high vacuum at 80 °C overnight to give 2-chloro-1,3-di-*tert*-butylimidazolium chloride as a colorless solid. Yield 79% (7.44 g, 29.60 mmol).



^{1}H NMR (400.13 MHz, $CDCl_3$): δ = 8.31 (s, 2 H, CH), 1.81 (s, 18 H, CH_3).

$^{13}C\{^1H\}$ NMR (100.62 MHz, $CDCl_3$): δ = 126.9 ($CClN_2$), 122.4 (CH), 64.7 ($C(CH_3)_2$), 29.1 (CH_3).

HRMS (ESI): m/z calculated for $[C_{11}H_{20}ClN_2]^+$ $(M)^+$ 215.13068, found 215.13095.

Elemental analysis: calculated (%) for $C_{11}H_{20}ClN_2$: C 52.60, H 8.03, N 11.15, found C 52.14, H 7.98, N 11.18.

IR (neat): $\tilde{\nu}$ = 1073 (m), 1053 (m), 1185 (vs), 1238 (m), 1273 (w), 1347 (m), 1377 (s), 1395 (s), 1456 (s), 1480 (m), 1557 (m), 1635 (m), 1681 (w), 2980 (m), 3094 (w), 3180 (m), 3364 (vs).

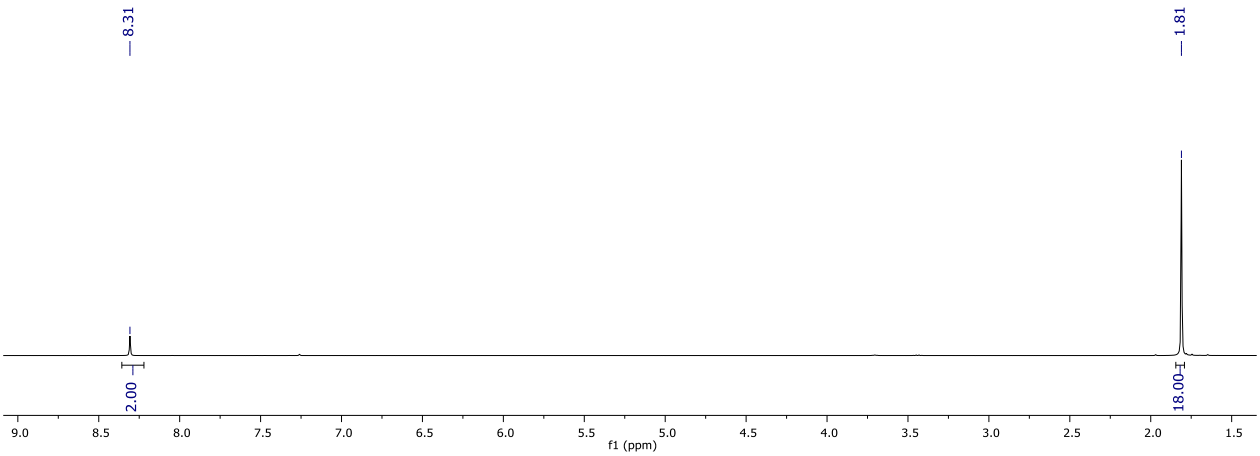


Figure S7: ^{1}H NMR spectrum (in $CDCl_3$, 300 K, 400.13 MHz) of 2-chloro-1,3-di-*tert*-butylimidazolium chloride.

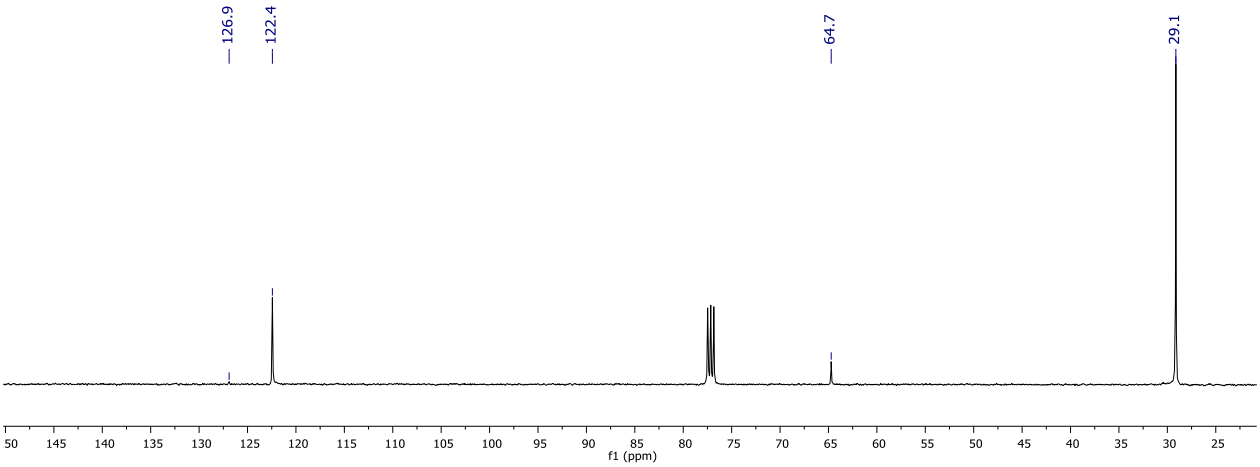
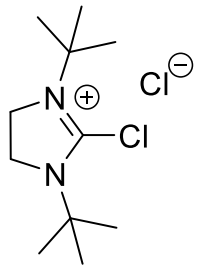


Figure S8: $^{13}C\{^{1}H\}$ NMR spectrum (in $CDCl_3$, 300 K, 100.62 MHz) of 2-chloro-1,3-di-*tert*-butylimidazolium chloride.

Synthesis of 2-chloro-1,3-di-*tert*-butylimidazolinium chloride: ASchlenk flask, connected to a bubbler, was charged with 1,3-di-*tert*-butylimidazolinium tetrafluoroborate (6.75 g, 25.00 mmol, 1.00 eq.), KO*t*Bu (0.14 g, 1.30 mmol, 0.05 eq.) and NaH (1.80 g, 75.00 mmol, 3.00 eq.). THF (75 mL) was added and the vigorously stirred mixture was heated to reflux overnight. The reaction mixture was allowed to cool to room temperature and the solids were filtered off. The volatiles of the filtrate were removed under reduced pressure to afford a colorless oil containing the free carbene. Distillation at 50 °C under reduced pressure gave the free carbene in pure form, which was then diluted in THF (50 mL) and treated with hexachloroethane (5.92 g, 25.00 mmol, 1.00 eq.). The reaction mixture was stirred at room temperature overnight. The resulting precipitate was collected on a frit and washed with Et_2O (3 x 20 mL). The solid was dried in high vacuum at 100 °C overnight to give the product as a colorless solid. Yield 86% (5.44 g, 21.50 mmol).



^{1}H NMR (400.13 MHz, $CDCl_3$): δ = 4.42 (s, 4 H, CH_2), 1.58 (s, 18 H, CH_3).

$^{13}C\{^1H\}$ NMR (100.60 MHz, $CDCl_3$): δ = 153.5 ($CClN_2$), 61.0 ($C(CH_3)_3$), 47.5 (CH_2), 28.8 (CH_3).

HRMS (ESI): m/z calculated for $[C_{11}H_{22}ClN_2]^+$ $(M)^+$ 217.14660, found 217.14631.

Elemental analysis: calculated (%) for $C_{11}H_{22}ClN_2$: C 52.18, H 8.76, N 11.06, found C 51.70, H 8.84, N 10.88.

IR (neat): $\tilde{\nu}$ = 1017 (m), 1056 (w), 1150 (w), 1196 (vs), 1232 (m), 1303 (m), 1379 (s), 1406 (m), 1462 (m), 1540 (s), 1578 (m), 1631 (s), 1656 (m), 2439 (w), 2494 (w), 2624 (m), 2683 (m), 2772 (m), 2977 (m), 3344 (m), 3410 (m).

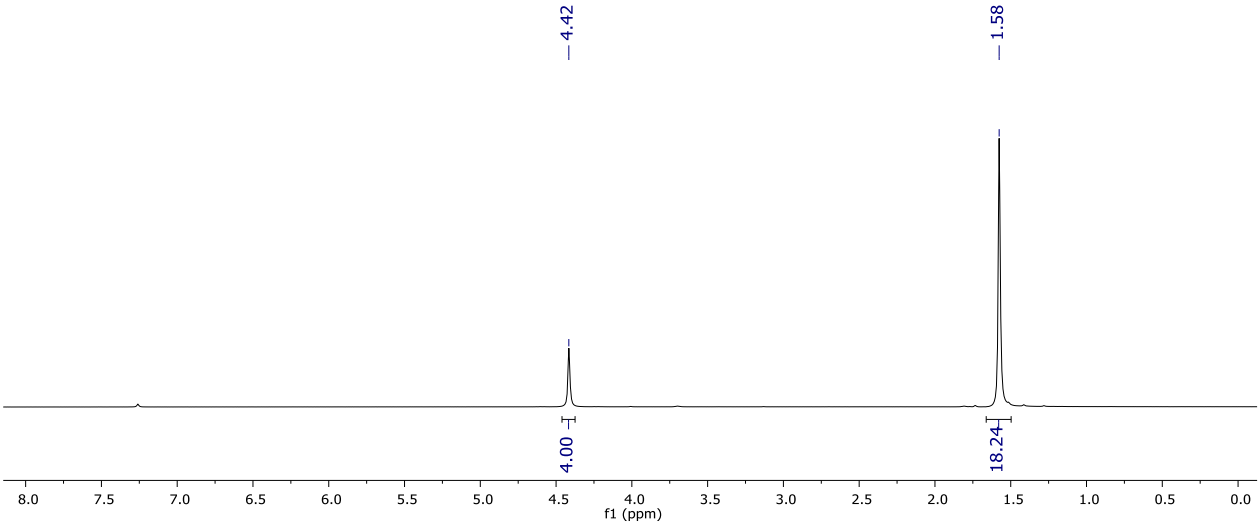


Figure S9: ^1H NMR spectrum (in $CDCl_3$, 300 K, 400.13 MHz) of 2-chloro-1,3-di-*tert*-butylimidazolinium chloride**.**

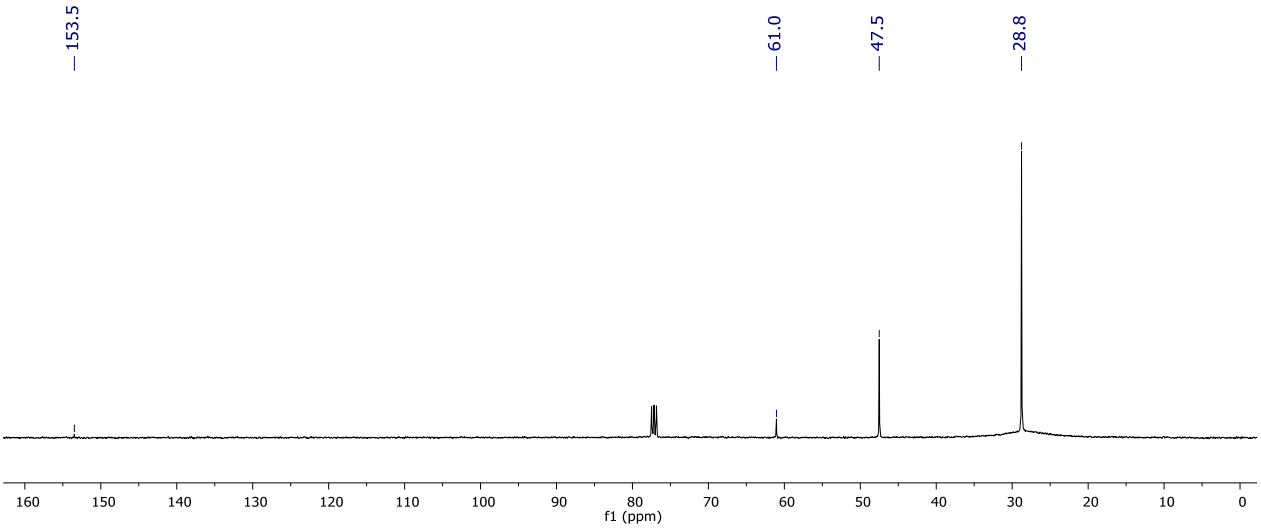


Figure S10: $^{13}C\{^1H\}$ NMR spectrum (in $CDCl_3$, 300 K, 100.60 MHz) of 2-chloro-1,3-di-*tert*-butylimidazolinium chloride.

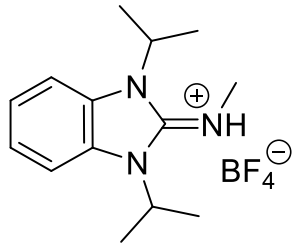
Synthesis of N-heterocyclic iminium salts **2**HBF_4-**3**HBF_4

The N-heterocyclic iminium salts were prepared according to the following general procedure (GP1), which follows the synthesis reported by Kunetskiy[2]: A Schlenk flask was charged with the 2-chloroazolium salt (1.00 eq.), anhydrous KF (6.00 eq.) and the amine RNH_2 or its hydrochloride salt RNH_3Cl. MeCN (3 mL per mmol of the 2-chloroazolium salt) was added and the resulting suspension was stirred at room temperature for the indicated period of time (see Table S1). $CHCl_3$ (5 mL per 1.00 mmol of the 2-chloroazolium salt) was added and the suspension was stirred for another 5 min at room temperature. The solid components were filtered off and the solution was transferred into a separation funnel. A diluted aq. solution of $NaBF_4$ (5.00 mmol per 1.00 mmol of the 2-chloroazolium salt) was added to the MeCN/$CHCl_3$ solution followed by vigorous shaking. The organic phase was separated and the aqueous phase was extracted once with a small amount of $CHCl_3$. The combined organic fractions were dried (anhydrous $MgSO_4$), filtered and the solvent was removed under reduced pressure to afford a colorless solid. After drying at 80 °C *in vacuo* overnight, the N-heterocyclic iminium salt was obtained with a purity of 99% according to NMR analysis.

Table S1*:* Ratio of reagents and conditions for synthesis of salts **2**HBF_4-**3**HBF_4.

Product	*Chlorosalt, eq.*	*RNH_2, eq.*	*RNH_3Cl, eq.*	*KF, eq.*	*Time, days*
2aHBF_4	1	-	2	6	2
2bHBF_4	1	3	-	6	3
3aHBF_4	1	-	3	6	3
3bHBF_4	1	3	-	6	7
3cHBF_4	1	3	-	6	3
3dHBF_4	1	3	-	6	3

Compound 2aHBF_4: Synthesis according to **GP1** starting from 2-chloro-1,3-diisopropylbenzimidazolium tetrafluoroborate (0.80 g, 2.46 mmol). Yield 90% (0.71 g, 2.22 mmol) as a colorless solid.



^{1}H NMR (400.03 MHz, $CDCl_3$): δ = 7.56 (m, 2H, aryl-H), 7.36 (m, 2H, aryl-H), 6.92 (q, $^3J_{HH}$ = 5.3 Hz, 1H, NH), 4.97 (hept, $^3J_{HH}$ = 6.9 Hz, 2H, $CH(CH_3)_2$), 3.35 (d, $^3J_{HH}$ = 5.0 Hz, 3H, NCH_3), 1.69 (d, $^3J_{HH}$ = 7.0 Hz, 12H, CH_3).

^{13}C{^{1}H} NMR (100.60 MHz, $CDCl_3$): δ = 150.3 (NCN_2), 128.9 (*ipso*-C), 124.4 (aryl-C), 113.7 (aryl-C), 50.2 ($CH(CH_3)_2$), 34.3 (NCH_3), 20.8 (CH3).

^{11}B NMR (128.35 MHz, $CDCl_3$): δ = -0.9.

^{11}B{^{1}H} NMR (128.35 MHz, $CDCl_3$): δ = -0.9.

^{19}F NMR (376.37 MHz, $CDCl_3$): δ = -152.7.

^{19}F{^{1}H} NMR (376.37 MHz, $CDCl_3$): δ = -152.7.

HRMS (ESI): m/z calculated for $[C_{14}H_{22}N_3]^+$ $(M)^+$ 232.18082, found 232.18049.
Elemental analysis: calculated (%) for $C_{14}H_{22}BF_4N_3$: C 52.69, H 6.95, N 13.17, found C 53.08, H 6.98, N 13.21

IR (neat): $\tilde{\nu}$ = 1003 (vs), 1069 (vs), 1118 (m), 1136 (m), 1166 (w), 1183 (w), 1300 (w), 1378 (m), 1395 (m), 1427 (m), 1479 (s), 1537 (m), 1603 (s), 1618 (s), 2948 (w), 2985 (w), 3359 (m).

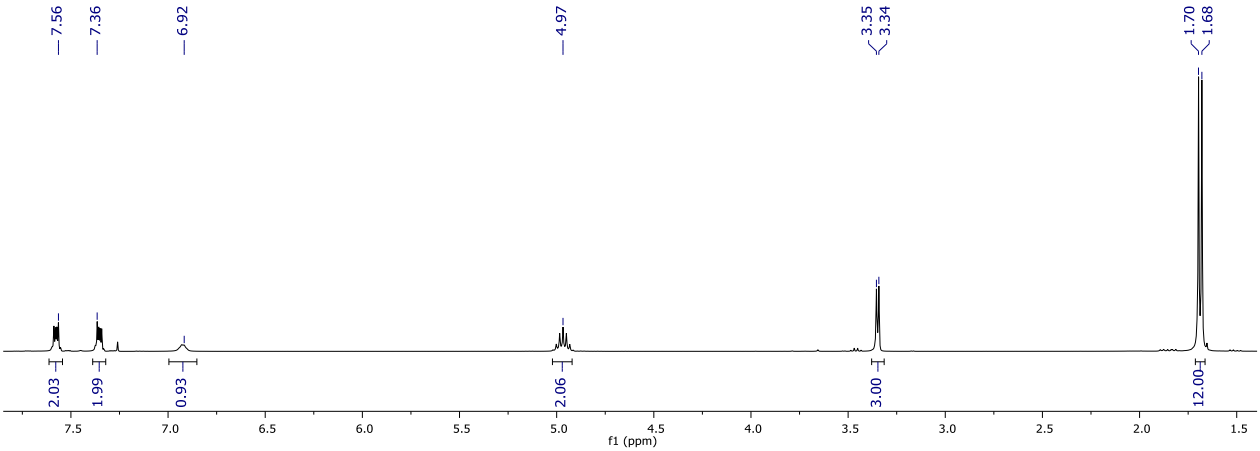


Figure S14: ^{1}H NMR spectrum (in $CDCl_3$, 300 K, 400.03 MHz) of **2a**HBF_4.

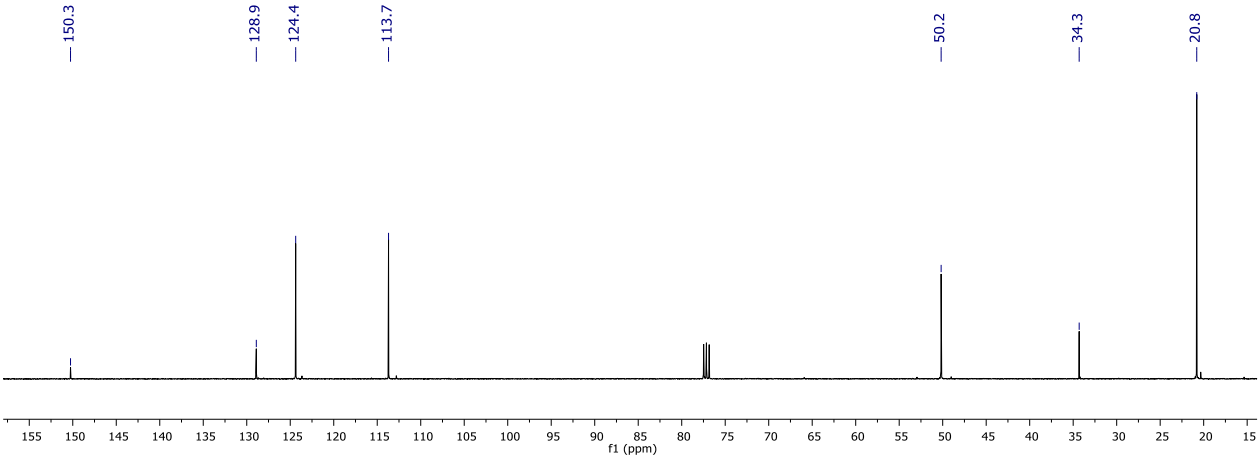


Figure S15: $^{13}C\{^{1}H\}$ NMR spectrum (in $CDCl_3$, 300 K, 100.60 MHz) of **2a**HBF_4.

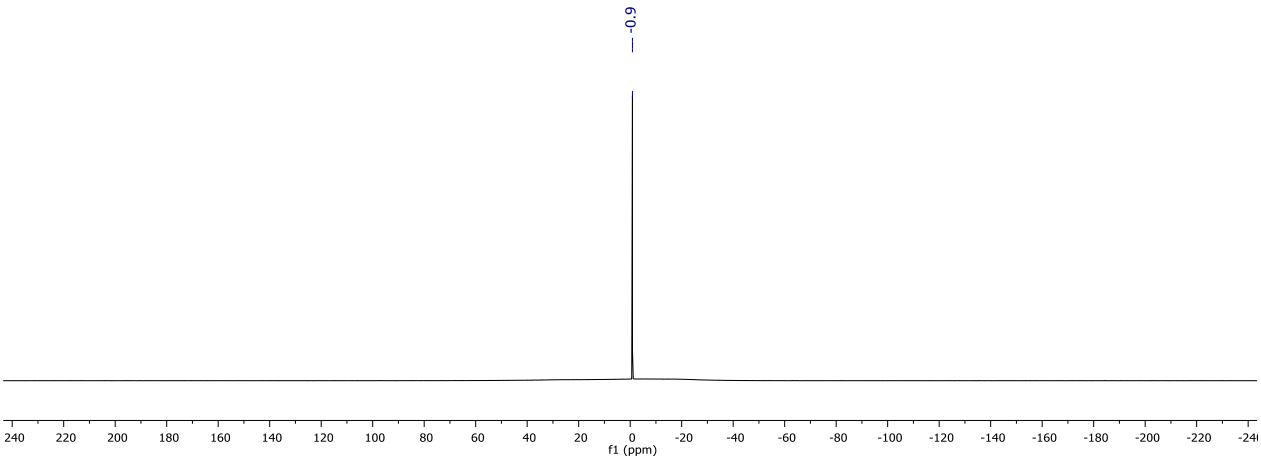


Figure S16: ^{11}B NMR spectrum (in $CDCl_3$, 300 K, 128.35 MHz) of **2a**HBF_4.

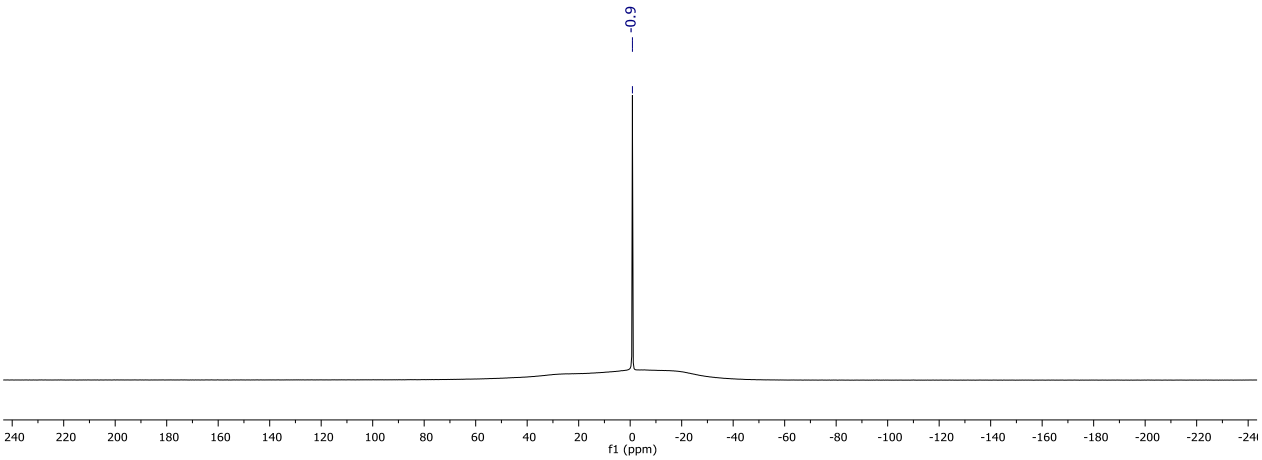


Figure S14: $^{11}B\{H\}$ NMR spectrum (in $CDCl_3$, 300 K, 128.35 MHz) of **2a**HBF_4.

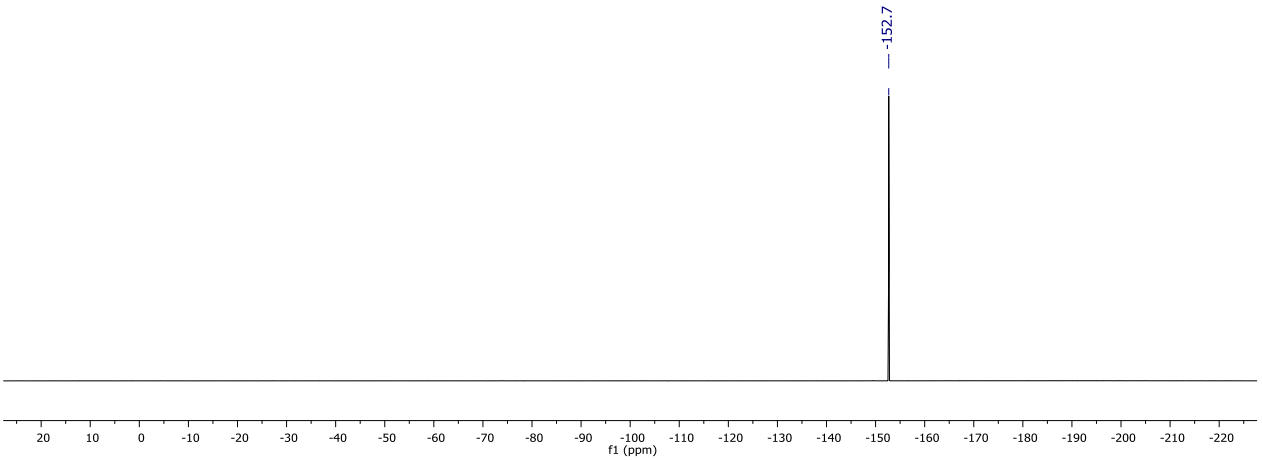


Figure S15: ^{19}F NMR spectrum (in $CDCl_3$, 300 K, 376.37 MHz) of **2a**HBF_4.

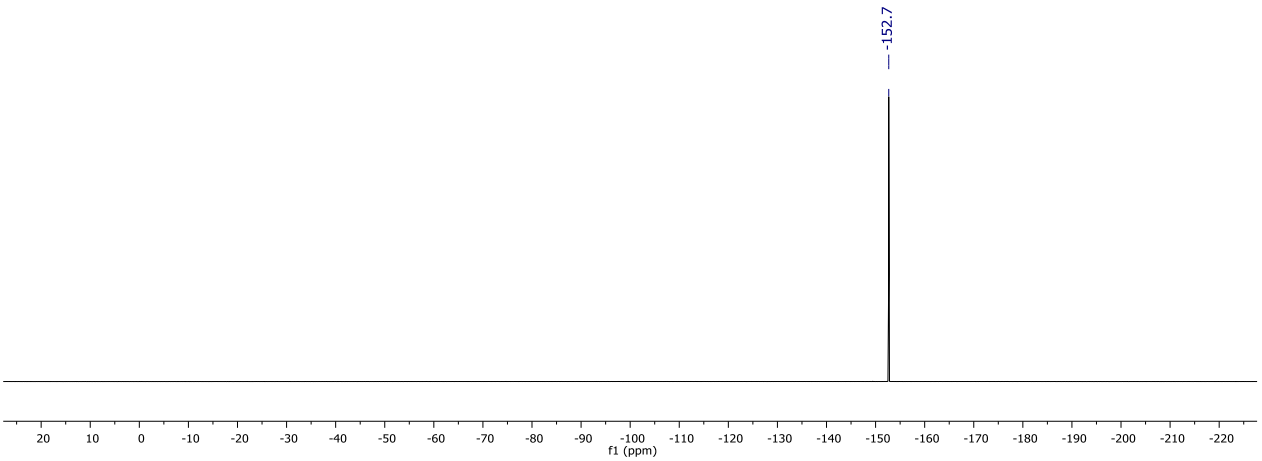
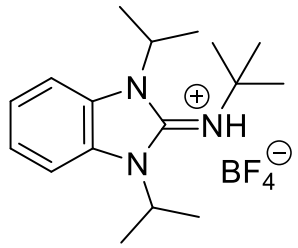


Figure S16: $^{19}F\{H\}$ NMR spectrum (in $CDCl_3$, 300 K, 376.37 MHz) of **2a**HBF_4.

Compound 2bHBF_4: Synthesis according to **GP1** starting from 2-chloro-1,3-diisopropylbenzimidazolium tetrafluoroborate (0.90 g, 2.77 mmol). Yield 82 % (0.82 g, 2.27 mmol) as a colorless solid.



^{1}H NMR (400.03 MHz, $CDCl_3$): δ = 7.77 (m, 2H, aryl-H), 7.51 (m, 2H, aryl-H), 5.70 (s, 1H, NH), 5.16 (hept, $^{3}J_{HH}$ = 7.0 Hz, 2H, $CH(CH_3)_2$), 1.70 (d, $^{3}J_{HH}$ = 7.0 Hz, 12H, CH_3), 1.41 (s, 9H, $C(CH_3)_3$).

^{13}C{^{1}H} NMR (100.60 MHz, $CDCl_3$): δ = 148.2 (NCN_2), 128.6 (*ipso*-C), 125.7 (aryl-C), 114.8 (aryl-C), 58.0 ($NC(CH_3)_3$), 51.3 ($CH(CH_3)_2$), 30.9 ($C(CH_3)_3$), 22.0 (CH_3).

^{11}B NMR (128.35 MHz, $CDCl_3$): δ = -0.9.

^{11}B{^{1}H} NMR (128.35 MHz, $CDCl_3$): δ = -0.9.

^{19}F NMR (376.37 MHz, $CDCl_3$): δ = -151.8.

^{19}F{^{1}H} NMR (376.37 MHz, $CDCl_3$): δ = -151.8.

HRMS (ESI): m/z calculated for $[C_{17}H_{28}N_3]^+$ $(M)^+$ 274.22777, found 274.22764.
Elemental analysis: calculated (%) for $C_{17}H_{28}BF_4N_3$: C 56.52, H 7.81, N 11.63, found C 56.55, H 7.73, N 11.52

IR (neat): $\tilde{\nu}$ = 1012 (vs), 1055 (vs), 1095 (s), 1150 (w), 1188 (m), 1226 (w), 1299 (w), 1377 (m), 1394 (m), 1406 (m), 1469 (s), 1520 (m), 2943 (w), 2978 (w), 3323 (w).

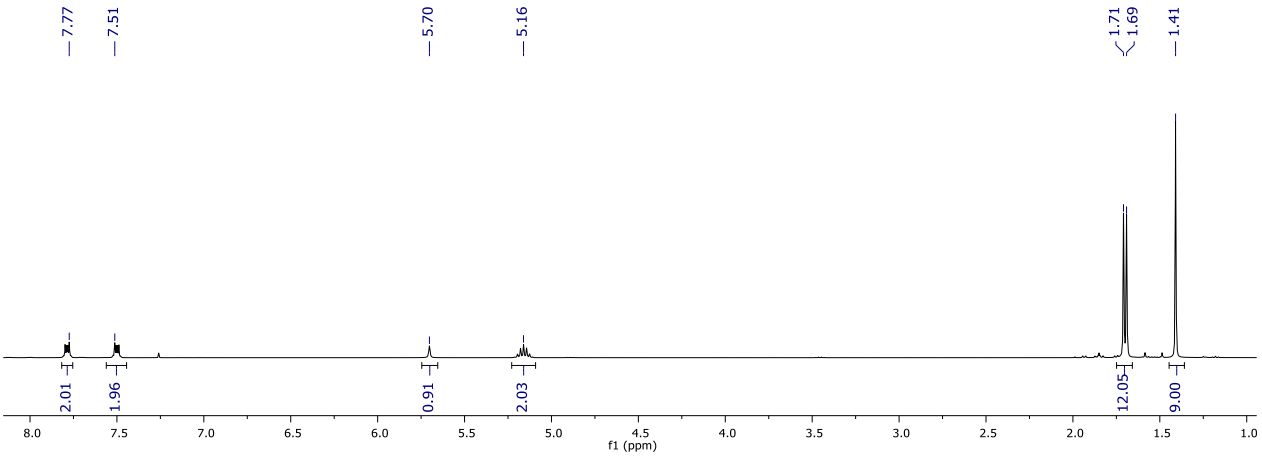


Figure S17: ^{1}H NMR spectrum (in $CDCl_3$, 300 K, 400.03 MHz) of **2b**HBF_4.

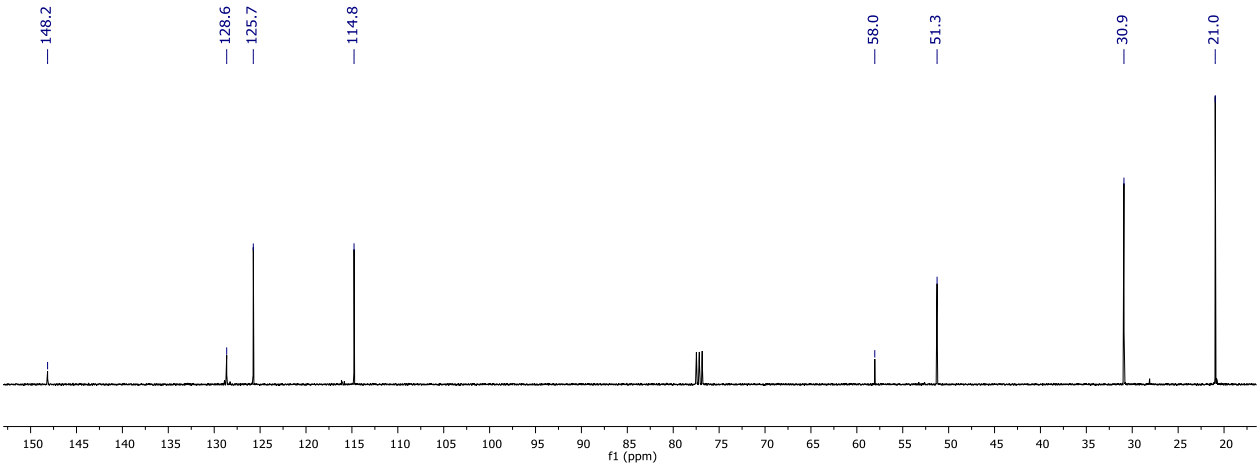


Figure S18: $^{13}C\{^{1}H\}$ NMR spectrum (in $CDCl_3$, 300 K, 100.60 MHz) of **2b**HBF_4.

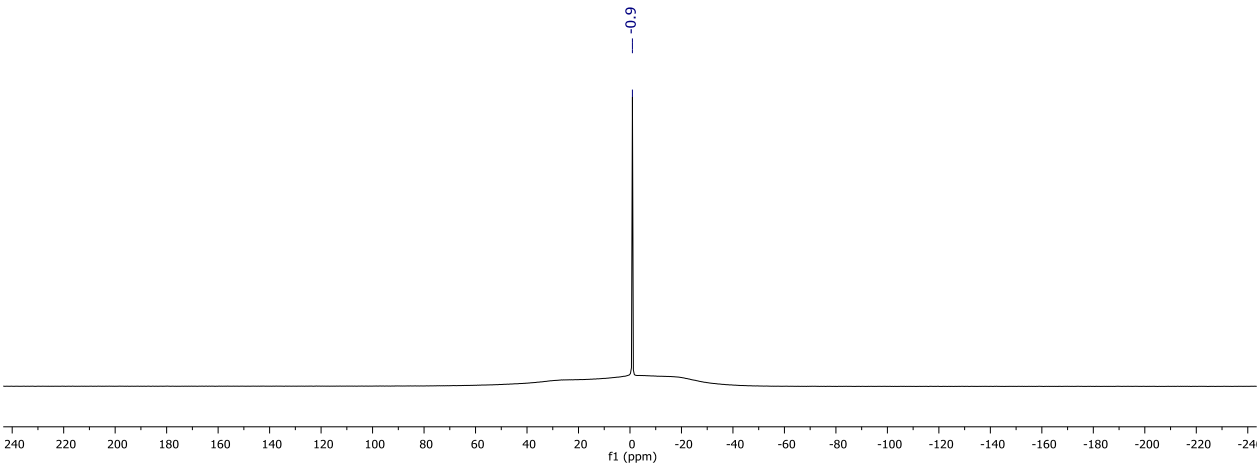


Figure S19: ^{11}B NMR spectrum (in $CDCl_3$, 300 K, 128.35 MHz) of **2b**HBF_4.

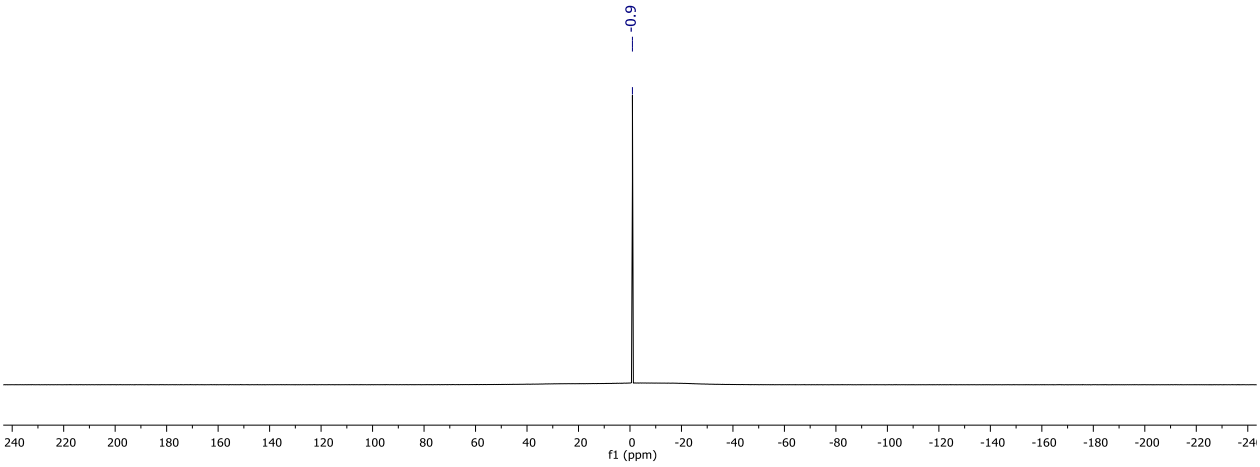


Figure S20: $^{11}B\{H\}$ NMR spectrum (in $CDCl_3$, 300 K, 128.35 MHz) of **2b**HBF_4.

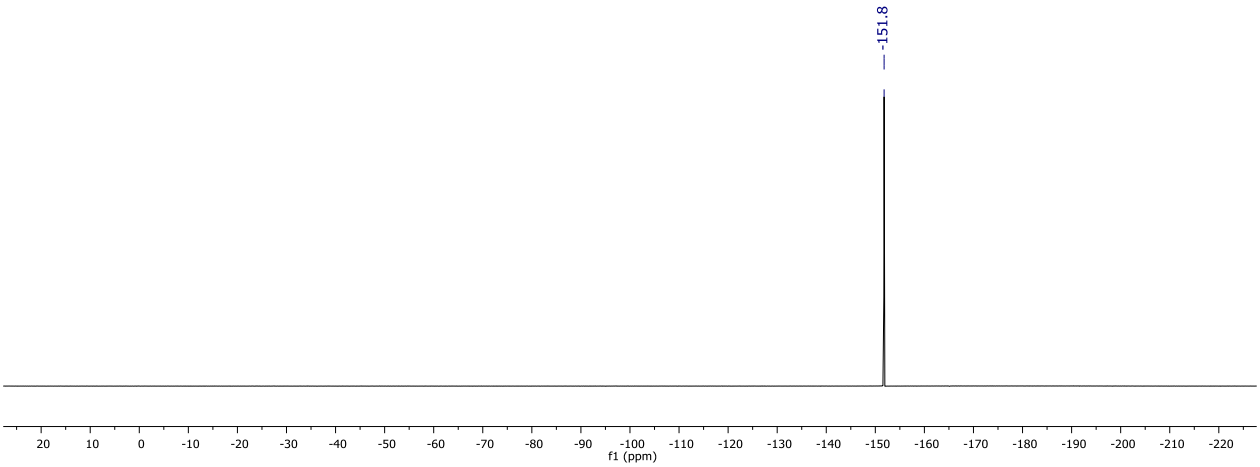


Figure S21: ^{19}F NMR spectrum (in $CDCl_3$, 300 K, 376.37 MHz) of **2b**HBF_4.

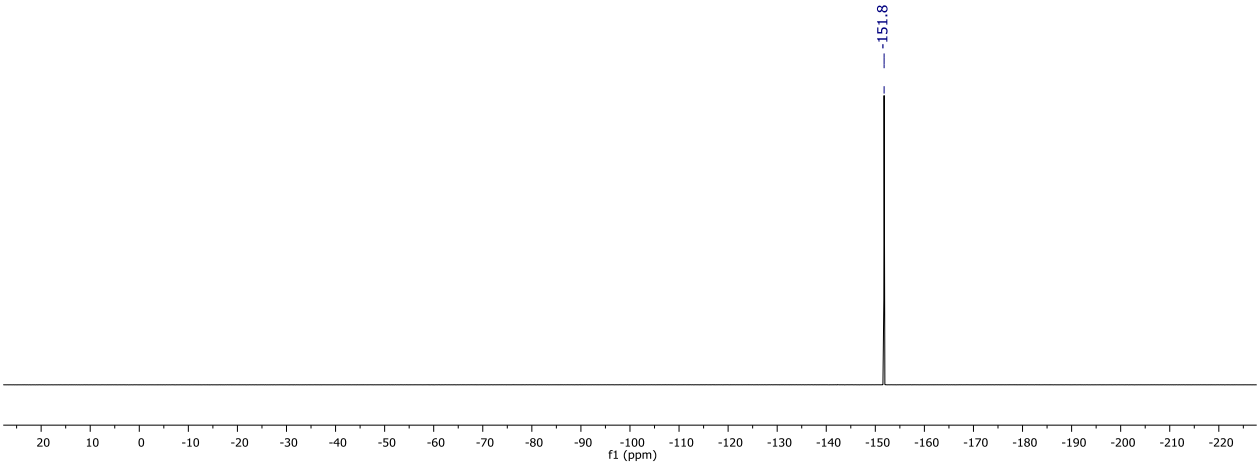
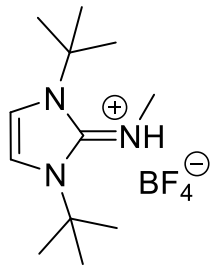


Figure S22: ^{19}F{H} NMR spectrum (in $CDCl_3$, 300 K, 376.37 MHz) of **2b**HBF_4.

Compound 3aHBF_4: Synthesis according to **GP1** starting from 2-chloro-1,3-di-*tert*-butylimidazolium chloride (1.42 g, 4.69 mmol). Yield 80 % (1.12 g, 3.77 mmol) as a colorless solid.



^{1}H NMR (400.03 MHz, $CDCl_3$): δ = 7.26 (s, 2H, CH), 4.15 (q, $^3J_{HH}$ = 5.2 Hz, 1H, NH), 2.90 (d, $^3J_{HH}$ = 5.1 Hz, 3H, NCH_3), 1.70 (s, 18H, $C(CH_3)_3$).

^{13}C{^{1}H} NMR (100.60 MHz, $CDCl_3$): δ = 144.9 (NCN_2), 116.8 (CH), 61.8 ($NC(CH_3)_3$), 37.1 (NCH_3), 30.0 ($C(CH_3)_3$).

^{11}B NMR (128.35 MHz, $CDCl_3$): δ = -1.0.

^{11}B{^{1}H} NMR (128.35 MHz, $CDCl_3$): δ = -1.0.

^{19}F NMR (376.39 MHz, $CDCl_3$): δ = -152.3.

^{19}F{^{1}H} NMR (376.39 MHz, $CDCl_3$): δ = -152.3.

HRMS (ESI): m/z calculated for $[C_{12}H_{24}N_3]^+$ $(M)^+$ 210.19647, found 210.19626.

Elemental analysis: calculated (%) for $C_{12}H_{24}BF_4N_3$: C 48.51, H 8.14, N 14.14, found C 48.40, H 8.00, N 14.15.

IR (neat): $\tilde{\nu}$ = 1027 (vs), 1050 (vs), 1192 (s), 1237 (w), 1248 (w), 1285 (w), 1332 (m), 1377 (m), 1406 (m), 1423 (m), 1446 (m), 1521 (m), 1573 (m), 2503 (w), 2981 (w), 3160 (w), 3382 (w).

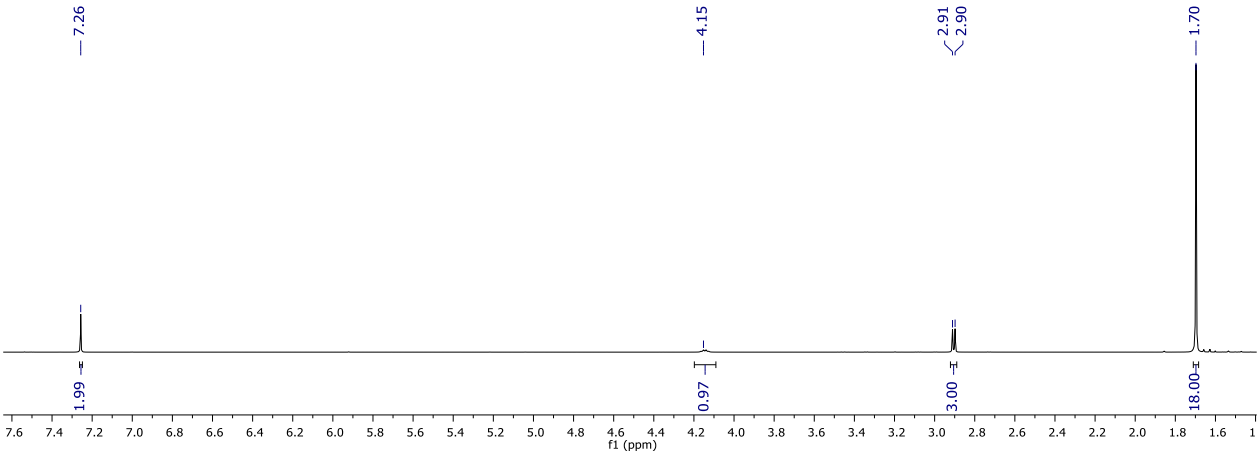


Figure S23: ^{1}H NMR spectrum (in $CDCl_3$, 300 K, 400.03 MHz) of **3a**HBF_4.

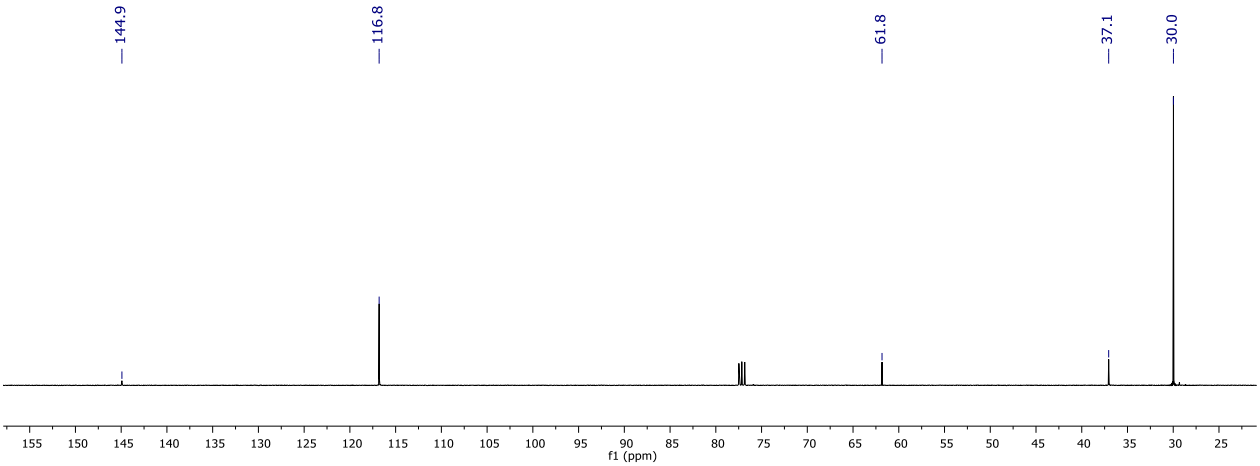


Figure S24: $^{13}C\{^{1}H\}$ NMR spectrum (in $CDCl_3$, 300 K, 100.60 MHz) of **3a**HBF_4.

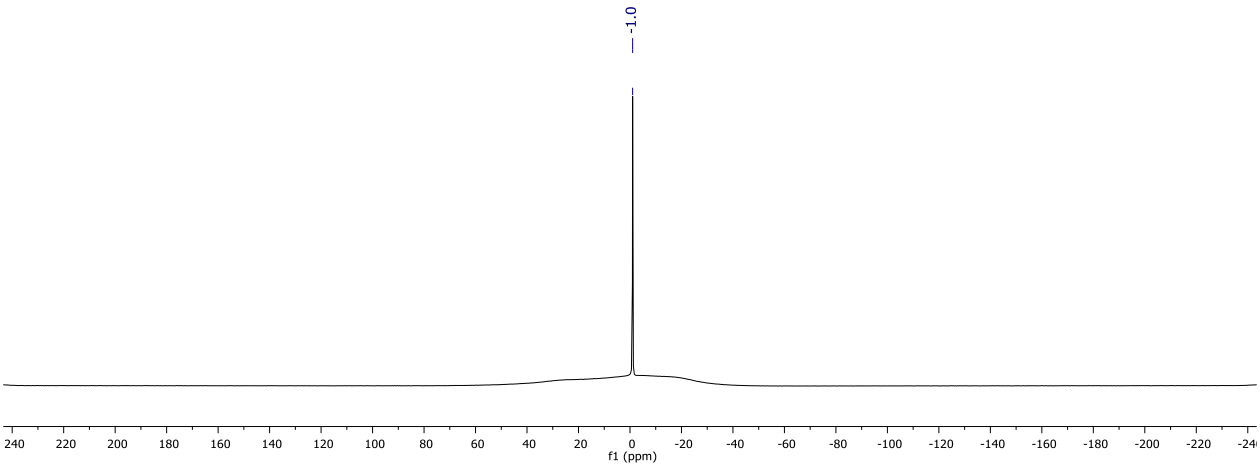


Figure S25: ^{11}B NMR spectrum (in $CDCl_3$, 300 K, 128.35 MHz) of **3a**HBF_4.

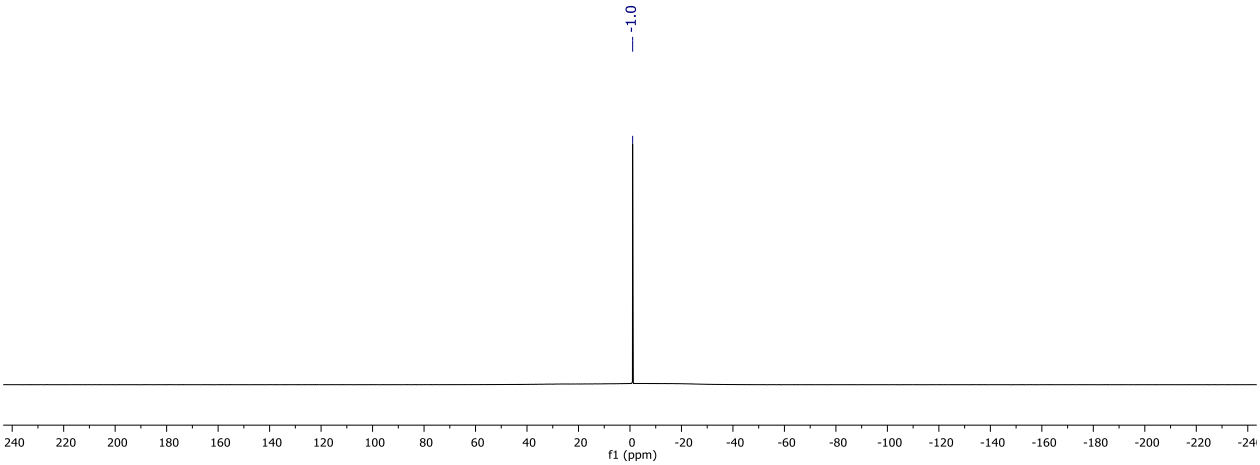


Figure S26: ^{11}B{H} NMR spectrum (in $CDCl_3$, 300 K, 128.35 MHz) of **3a**HBF_4.

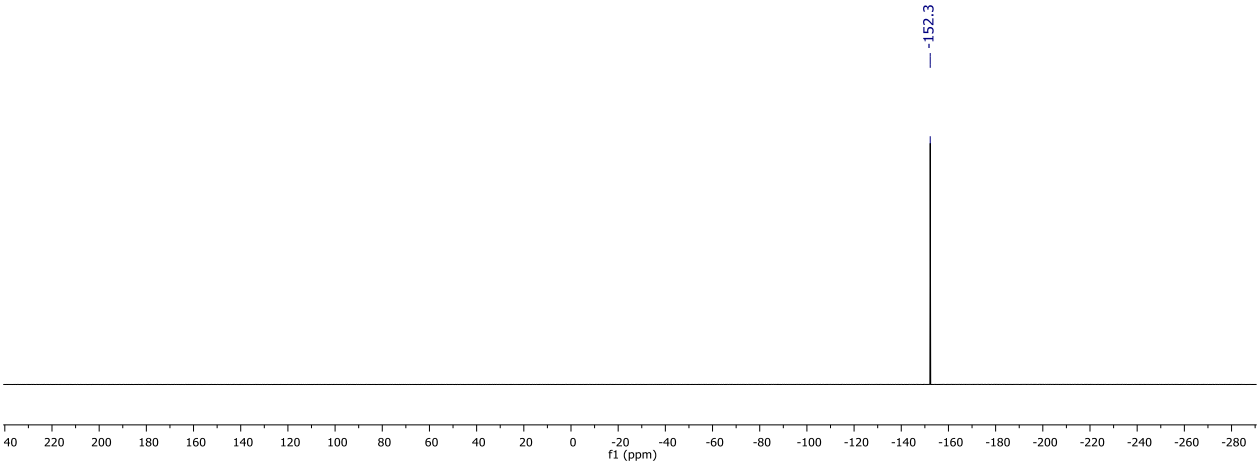


Figure S27: ^{19}F NMR spectrum (in $CDCl_3$, 300 K, 376.39 MHz) of **3a**HBF_4.

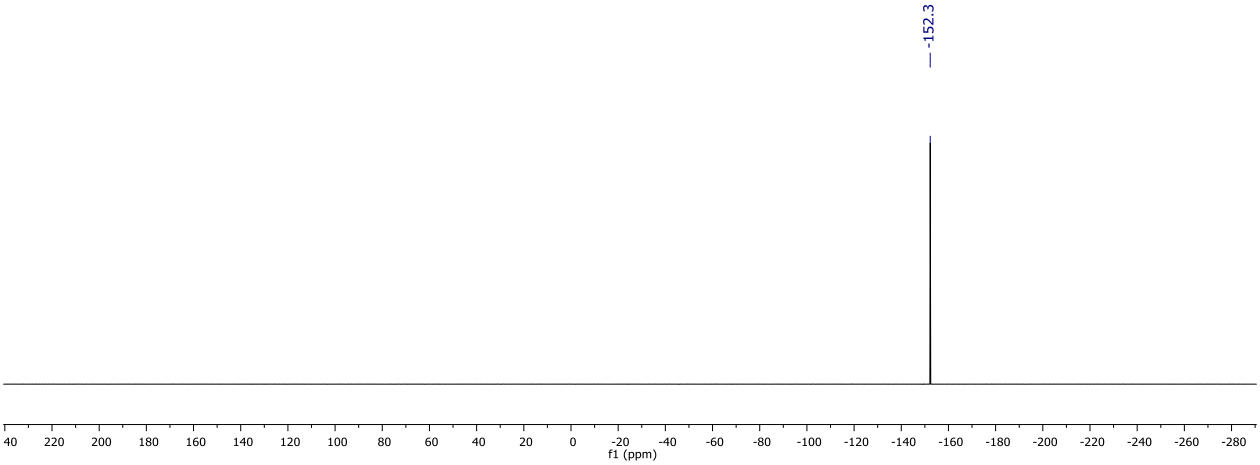
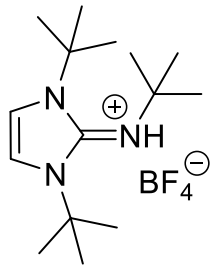


Figure S28: $^{19}F\{H\}$ NMR spectrum (in $CDCl_3$, 300 K, 376.39 MHz) of **3a**HBF_4.

Compound 3bHBF_4: Synthesis according to **GP1** starting from 2-chloro-1,3-di-*tert*-butylimidazolium chloride (1.59 g, 6.33 mmol). Yield 92 % (1.98 g, 5.84 mmol) as a colorless solid.



^{1}H NMR (400.03 MHz, $CDCl_3$): δ = 7.37 (s, 2H, CH), 3.67 (s, 1H, NH), 1.68 (s, 18H, $C(CH_3)_3$), 1.27 (s, 9H, CH_3).

^{13}C{^{1}H} NMR (100.60 MHz, $CDCl_3$): δ = 142.6 (NCN_2), 118.4 (CH), 63.1 (2x$NC(CH_3)_3$), 56.8 ($NC(CH_3)_3$), 30.6 (6xCH_3), 30.3 (3xCH3).

^{11}B NMR (128.35 MHz, $CDCl_3$): δ = -1.1.

^{11}B{^{1}H} NMR (128.35 MHz, $CDCl_3$): δ = -1.1.

^{19}F NMR (376.39 MHz, $CDCl_3$): δ = -150.9.

^{19}F{^{1}H} NMR (376.39 MHz, $CDCl_3$): δ = -150.9.

HRMS (ESI): m/z calculated for $[C_{15}H_{30}N_3]^+$ $(M)^+$ 252.24342, found 252.24407.
IR (neat): $\tilde{\nu}$ = 1030 (vs), 1046 (vs), 1082 (s), 1096 (s), 1191 (s), 1236 (m), 1283 (w), 1318 (w), 1374 (m), 1393 (w), 1405 (w), 1429 (m), 1454 (m), 1483 (m), 1580 (m), 1622 (w), 2985 (w), 3209 (w), 3380 (w).

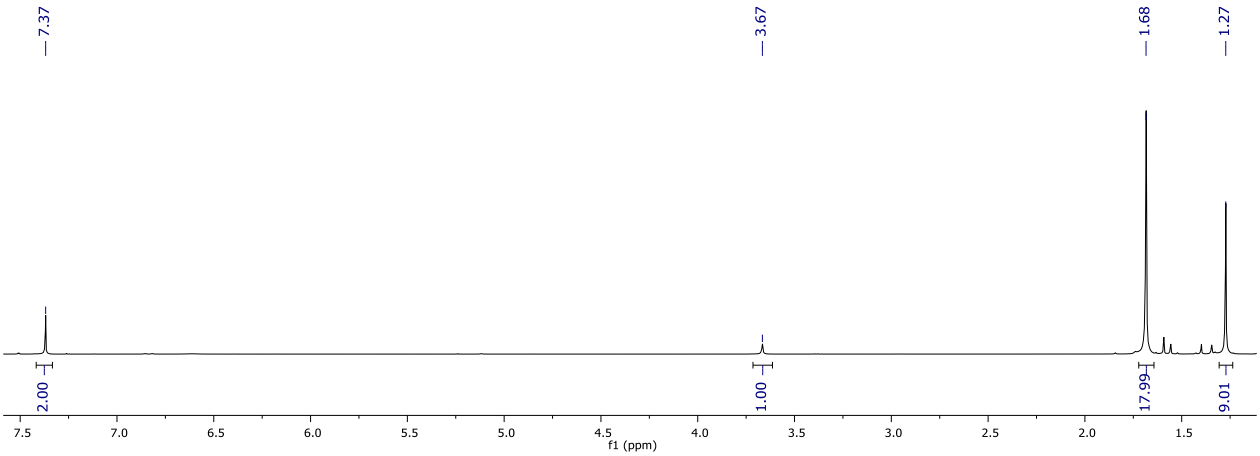


Figure S29: ^{1}H NMR spectrum (in $CDCl_3$, 300 K, 400.03 MHz) of **3b**HBF_4.

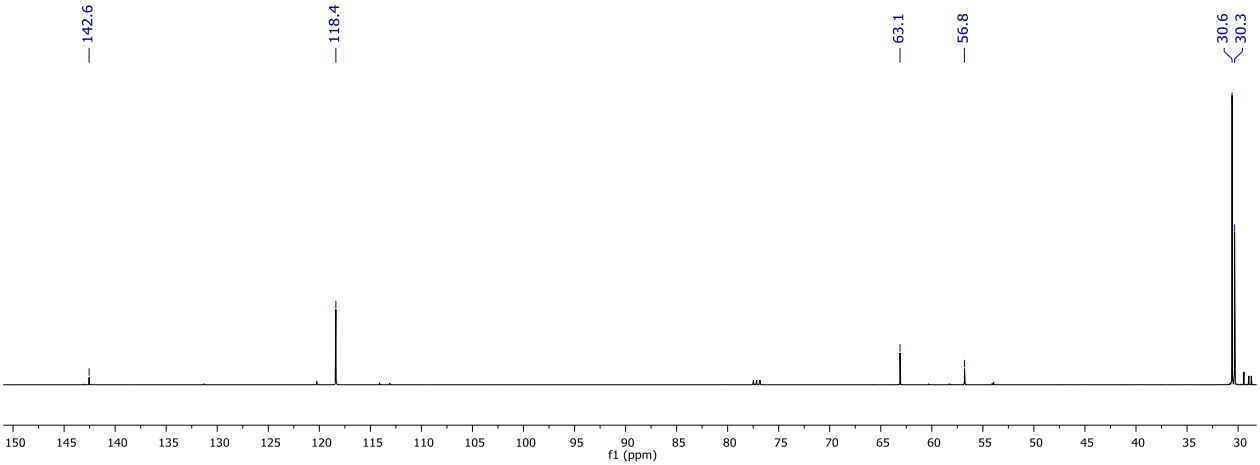


Figure S30: $^{13}C\{^{1}H\}$ NMR spectrum (in $CDCl_3$, 300 K, 100.60 MHz) of **3b**HBF_4.

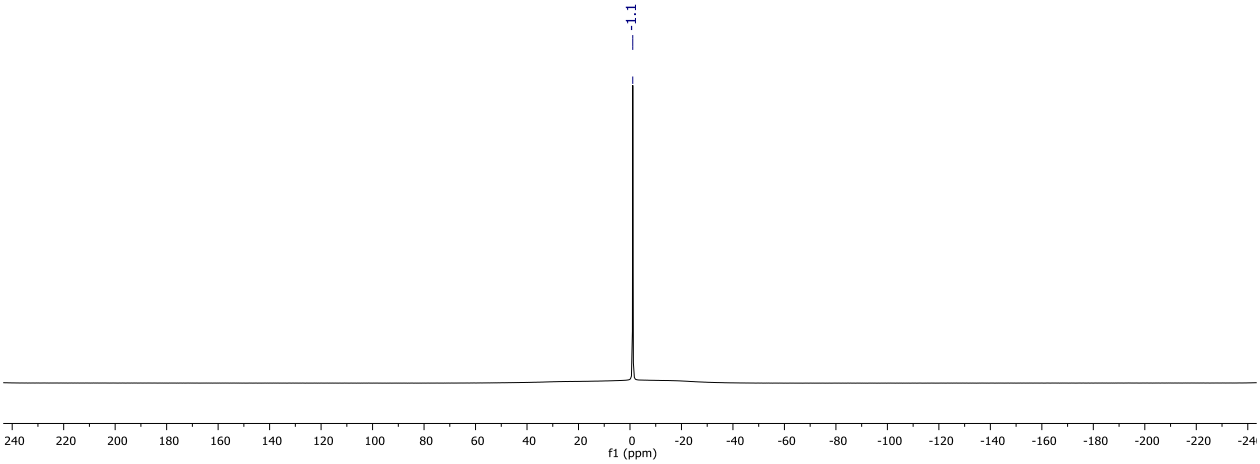


Figure S31: ^{11}B NMR spectrum (in $CDCl_3$, 300 K, 128.35 MHz) of **3b**HBF_4.

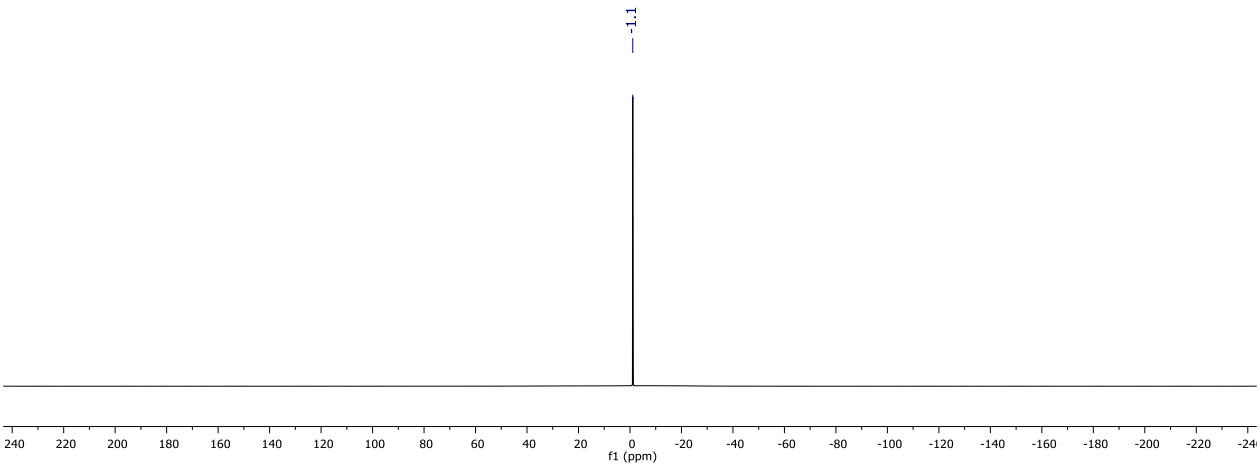


Figure S32: $^{11}B\{H\}$ NMR spectrum (in $CDCl_3$, 300 K, 128.35 MHz) of **3b**HBF_4.

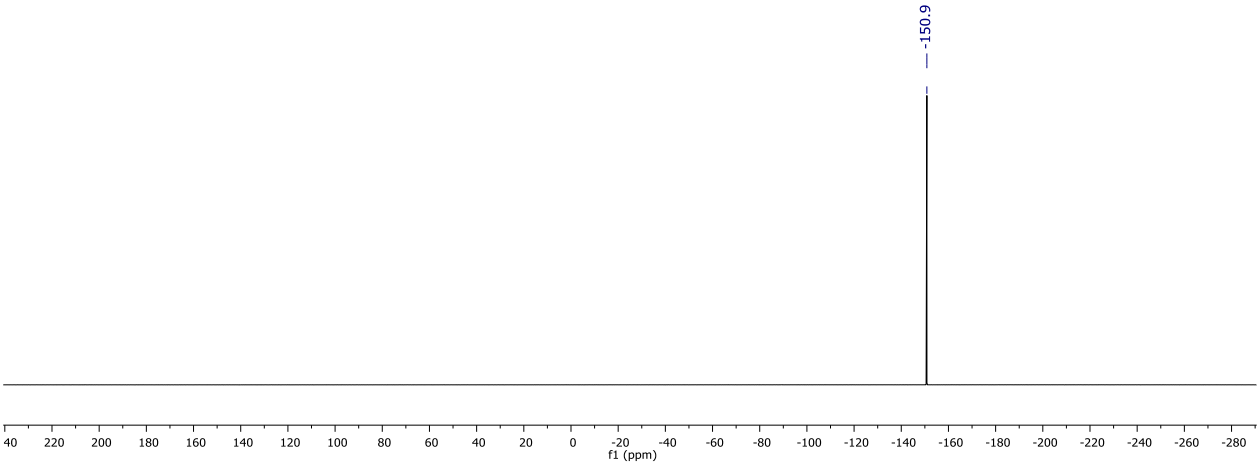


Figure S33: ^{19}F NMR spectrum (in $CDCl_3$, 300 K, 376.39 MHz) of **3b**HBF_4.

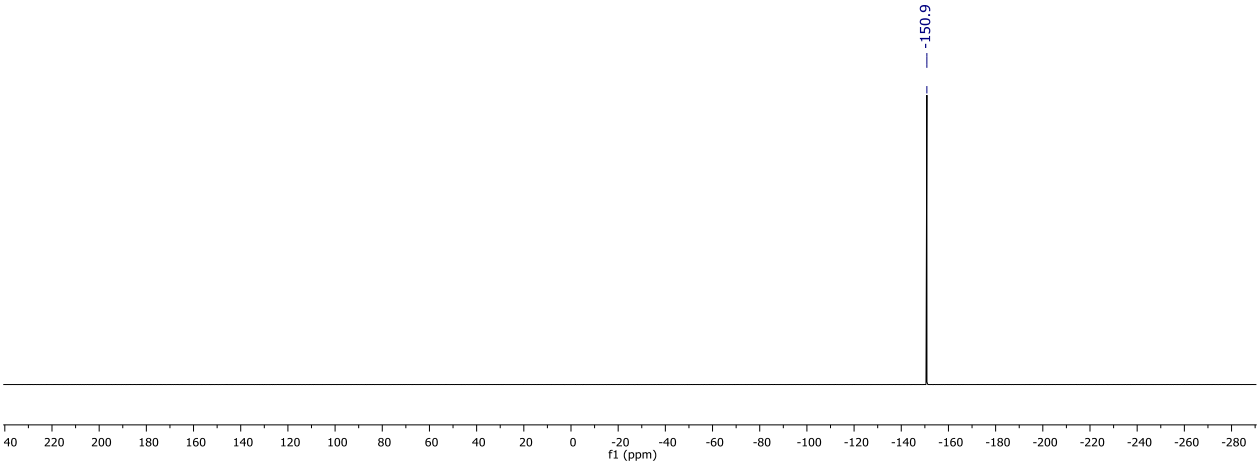
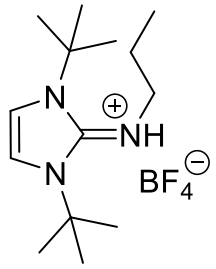


Figure S34: $^{19}F\{H\}$ NMR spectrum (in $CDCl_3$, 300 K, 376.39 MHz) of **3b**HBF_4.

Compound 3cHBF_4: Synthesis according to **GP1** starting from 2-chloro-1,3-di-*tert*-butylimidazolium chloride (1.60 g, 6.37 mmol). Yield 84% (1.73 g, 5.32 mmol) as a colorless solid.



^{1}H NMR (400.03 MHz, $CDCl_3$): δ = 7.22 (s, 2H, CH), 3.87 (t, $^3J_{HH}$ = 5.9 Hz, 1H, NH), 2.94 (q, $^3J_{HH}$ = 6.8 Hz, 2H, NCH_2), 1.68 (m, 2H, CH_2), 1.61 (s, 18H, $C(CH_3)_3$), 0.89 (t, $^3J_{HH}$ = 7.4 Hz, 3H, CH_3).

^{13}C{^{1}H} NMR (100.60 MHz, $CDCl_3$): δ = 143.5 (NCN_2), 116.9 (CH), 61.6 ($NC(CH_3)_3$), 51.9 (NCH_2CH_2), 29.5 ($C(CH_3)_3$), 22.3 (CH_2), 10.9 (CH_3).

^{11}B NMR (128.35 MHz, $CDCl_3$): δ = -1.1.

^{11}B{^{1}H} NMR (128.35 MHz, $CDCl_3$): δ = -1.1.

^{19}F NMR (376.37 MHz, $CDCl_3$): δ = -151.6.

^{19}F{^{1}H} NMR (376.37 MHz, $CDCl_3$): δ = -151.6.

HRMS (ESI): m/z calculated for $[C_{14}H_{28}N_3]^+$ $(M)^+$ 238.2278, found 238.2286.
Elemental analysis: calculated (%) for $C_{14}H_{28}BF_4N_3$: C 51.71, H 8.68, N 12.92, found C 51.35, H 8.29, N 12.76.
IR (neat): $\tilde{\nu}$ = 1031 (vs), 1045 (vs), 1192 (s), 1240 (m), 1283 (w), 1330 (w), 1375 (m), 1406 (w), 1428 (w), 1462 (m), 1481 (m), 1509 (w), 1578 (w), 1603 (w), 2880 (w), 2980 (w), 3365 (w).

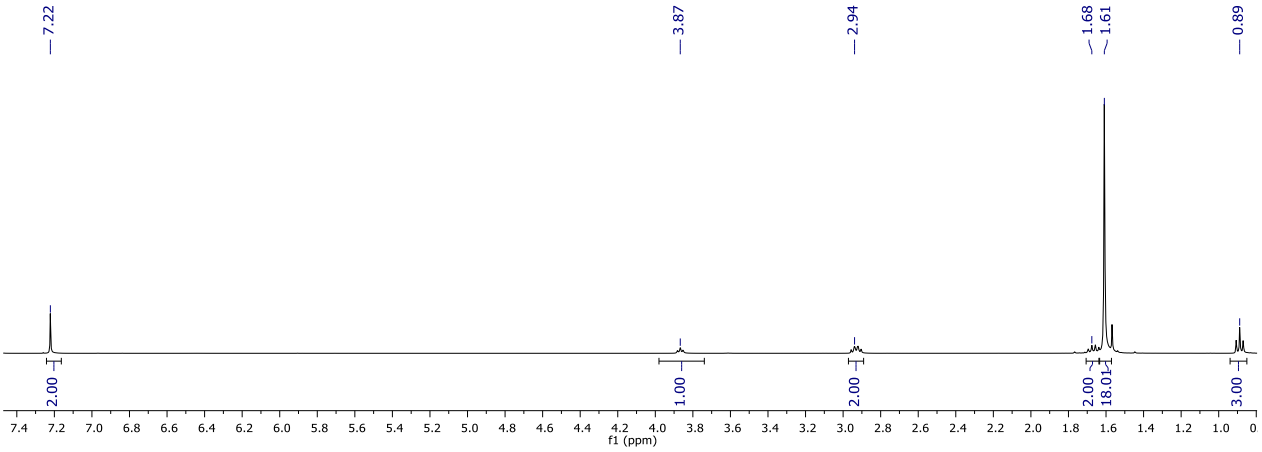


Figure S35: ^{1}H NMR spectrum (in $CDCl_3$, 300 K, 400.03 MHz) of **3c**HBF_4.

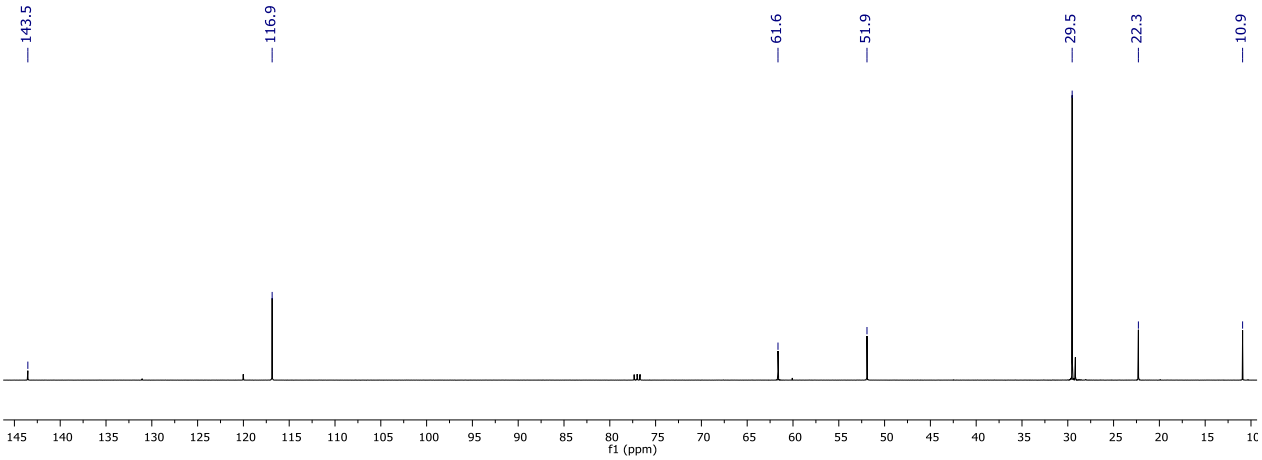


Figure S36: $^{13}C\{^{1}H\}$ NMR spectrum (in $CDCl_3$, 300 K, 100.60 MHz) of **3c**HBF_4.

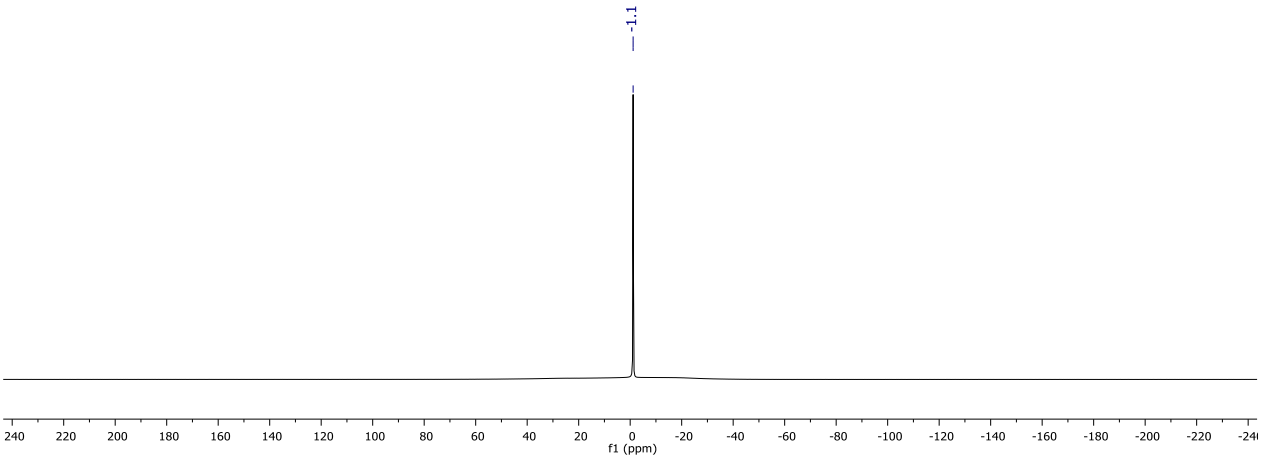


Figure S37: ^{11}B NMR spectrum (in $CDCl_3$, 300 K, 128.35 MHz) of **3c**HBF_4.

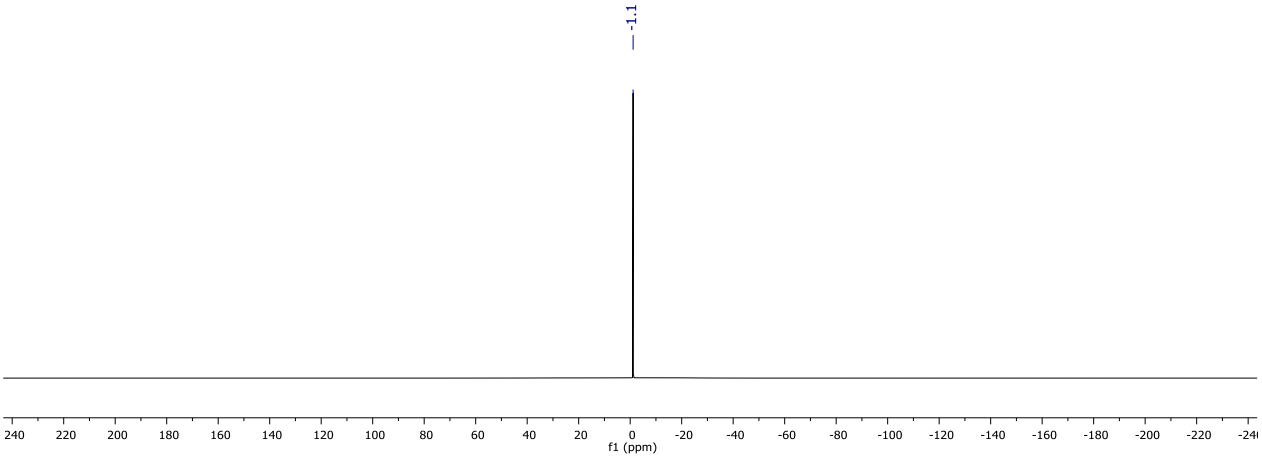


Figure S38: $^{11}B\{H\}$ NMR spectrum (in $CDCl_3$, 300 K, 128.35 MHz) of **3c**HBF_4.

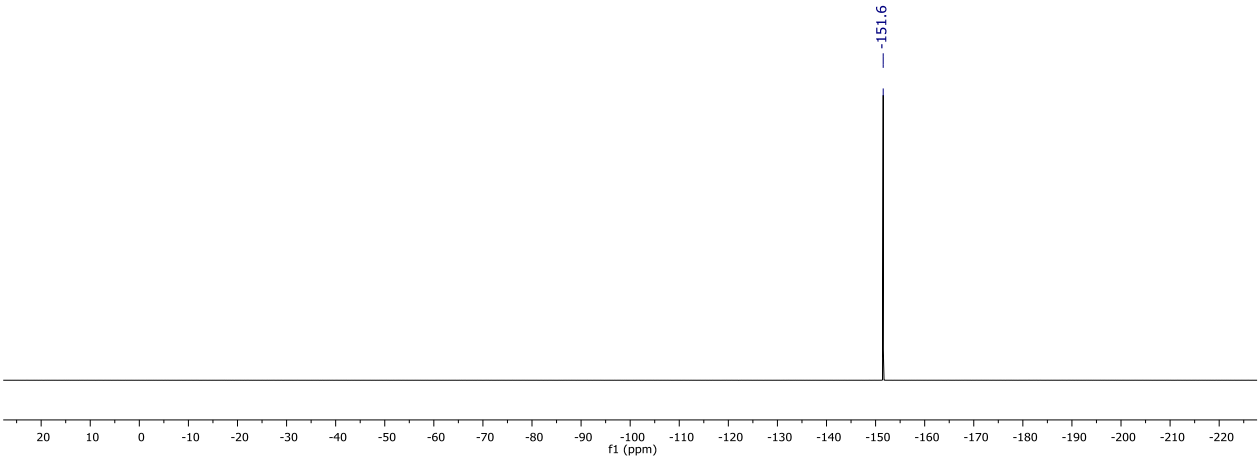


Figure S39: ^{19}F NMR spectrum (in $CDCl_3$, 300 K, 376.37 MHz) of **3c**HBF_4.

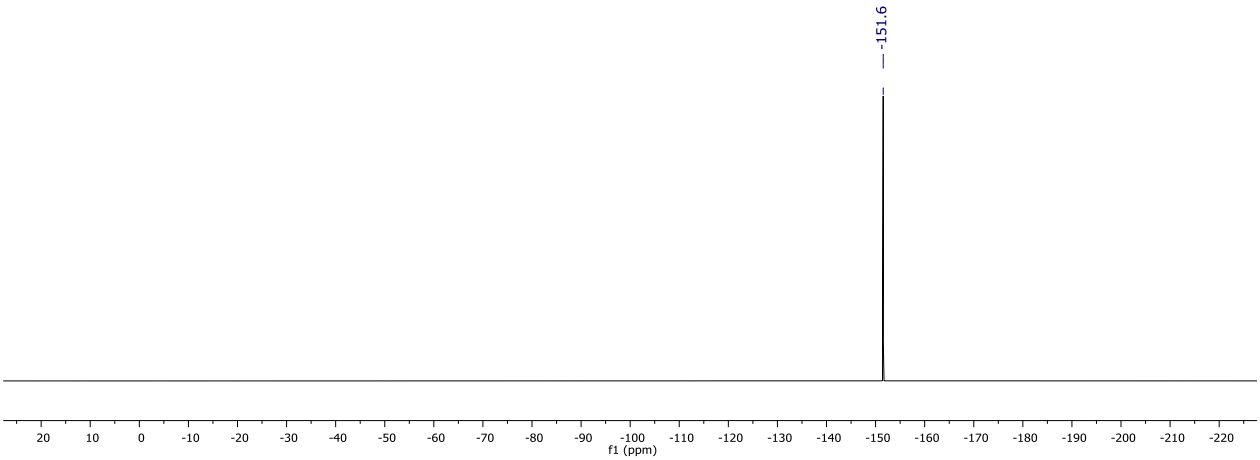
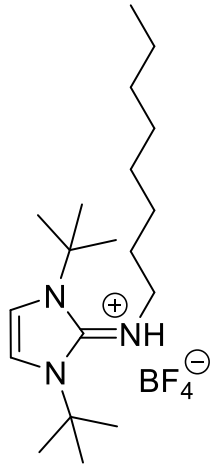


Figure S40: ^{19}F{H} NMR spectrum (in $CDCl_3$, 300 K, 376.37 MHz) of **3c**HBF_4.

Compound 3dHBF_4: Synthesis according to **GP1** starting from 2-chloro-1,3-di-*tert*-butylimidazolium chloride (0.80 g, 3.18 mmol). Yield 87% (1.09 g, 2.76 mmol) as a colorless oil.



^{1}H NMR (400.03 MHz, $CDCl_3$): δ = 7.24 (s, 2H, CH), 3.84 (s, 1H, NH), 3.06 (t, $^3J_{HH}$ = 7.5 Hz, 2H, NCH_2), 1.74 (s, 18H, $C(CH_3)_3$), 1.47 (s, 2H, CH_2), 1.27 (m, 10H, 5 x CH_2), 0.88 (t, $^3J_{HH}$ = 6.5 Hz, 3H, CH_3).

^{13}C{^{1}H} NMR (100.60 MHz, $CDCl_3$): δ = 144.3 (NCN_2), 117.1 (CH), 62.3 ($NC(CH_3)_3$), 50.8 (NCH_2), 31.9 (CH_2), 30.2 ($C(CH_3)_3$), 29.7 (CH_2), 29.5 (CH_2), 29.3 (CH_2), 27.0 (CH_2), 22.8 (CH_2), 14.2 (CH_3).

^{11}B NMR (128.38 MHz, $CDCl_3$): δ = -1.1.

^{11}B{^{1}H} NMR (128.38 MHz, $CDCl_3$): δ = -1.1.

^{19}F NMR (376.37 MHz, $CDCl_3$): δ = -151.6.

^{19}F{^{1}H} NMR (376.37 MHz, $CDCl_3$): δ = -151.6.

HRMS (ESI): m/z calculated for $[C_{19}H_{38}N_3]^+$ $(M)^+$ 308.3060, found 308.3066.

IR (neat): $\tilde{\nu}$ = 1033 (vs), 1051 (vs), 1191 (s), 1238 (m), 1284 (w), 1330 (w), 1377 (m), 1407 (w), 1461 (m), 1491 (m), 1576 (m), 1649 (w), 2856 (m), 2927 (s), 3198 (w), 3366 (w).

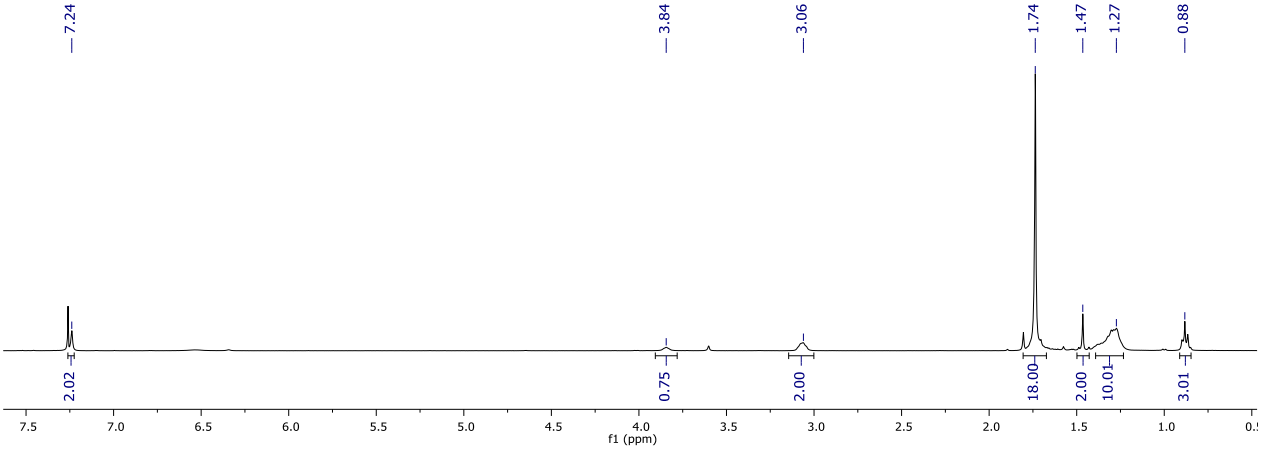


Figure S41: ^{1}H NMR spectrum (in $CDCl_3$, 300 K, 400.03 MHz) of **3d**HBF_4.

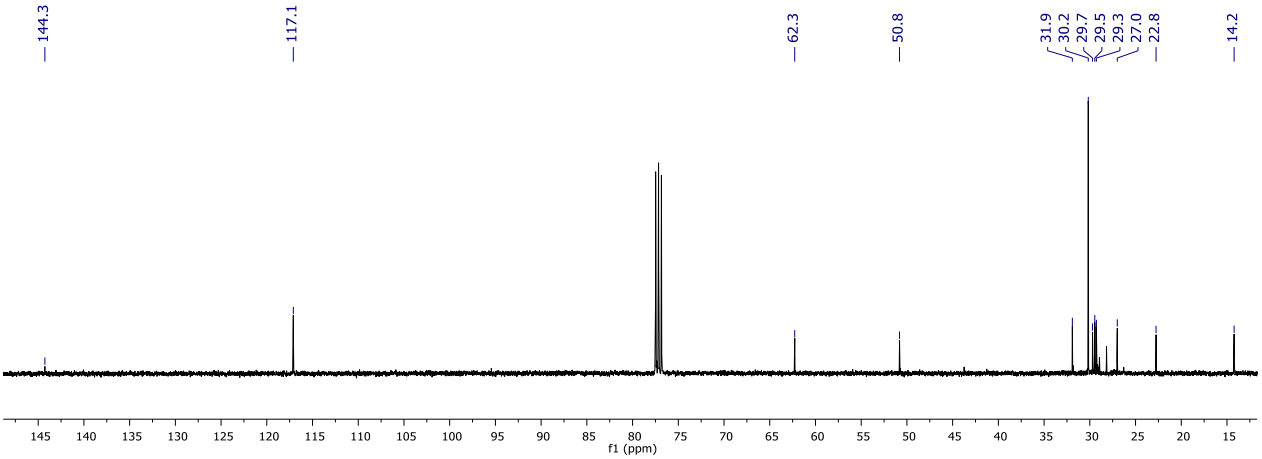


Figure S42: $^{13}C\{^{1}H\}$ NMR spectrum (in $CDCl_3$, 300 K, 100.60 MHz) of **3d**HBF_4.

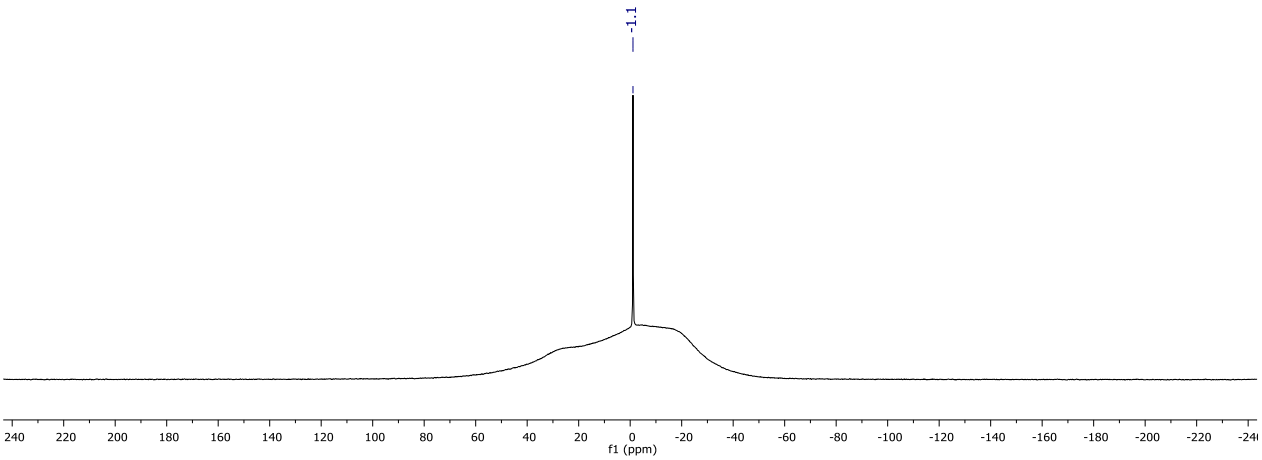


Figure S43: ^{11}B NMR spectrum (in $CDCl_3$, 300 K, 128.38 MHz) of **3d**HBF_4.

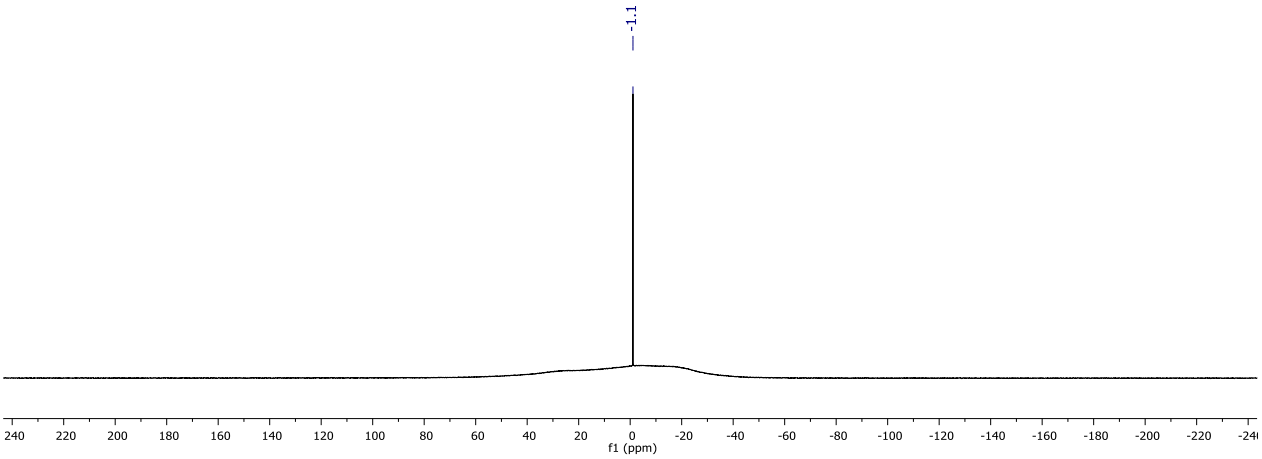


Figure S44: ^{11}B{H} NMR spectrum (in $CDCl_3$, 300 K, 128.38 MHz) of **3d**HBF_4.

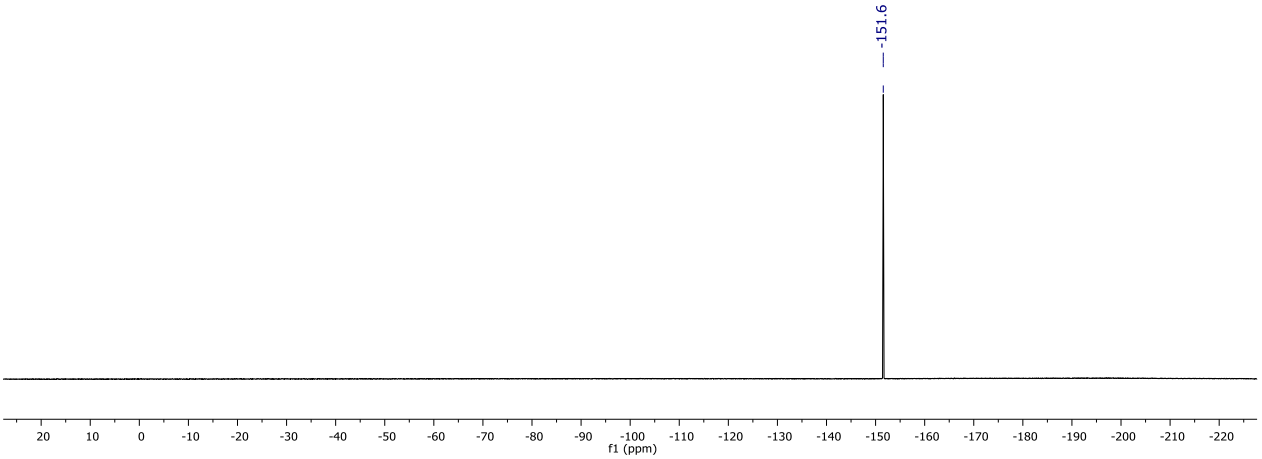


Figure S45: ^{19}F NMR spectrum (in $CDCl_3$, 300 K, 376.37 MHz) of **3d**HBF_4.

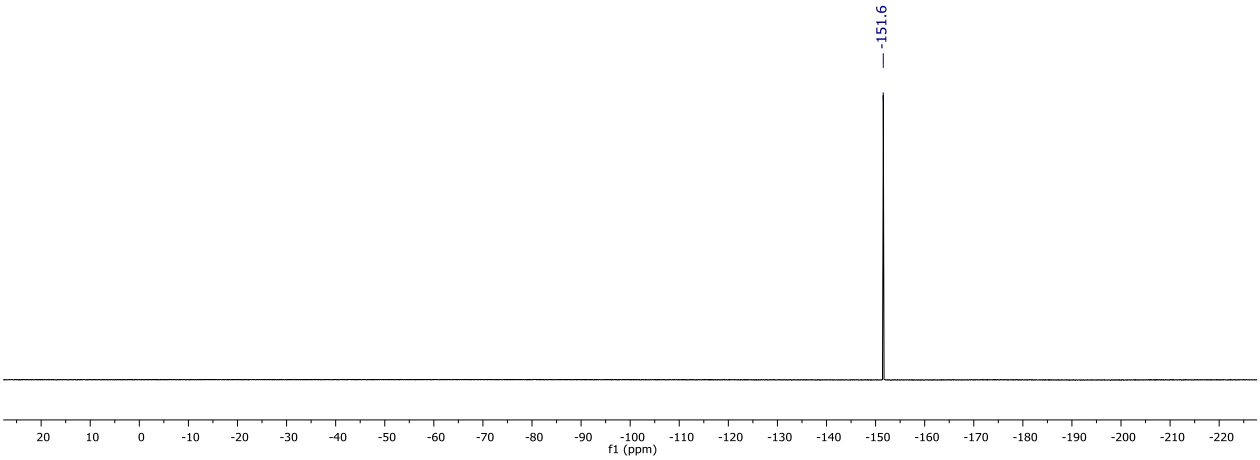
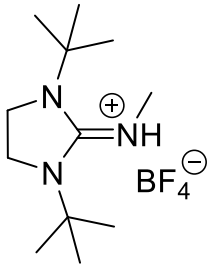


Figure S46: $^{19}F\{H\}$ NMR spectrum (in $CDCl_3$, 300 K, 376.37 MHz) of **3d**HBF_4.

Synthesis of 1,3-di-*tert*-butylimidazolidin-2-iminium salt **5**HBF_4

Compound 5HBF_4: Anhydrous triethylamine (1.60 g, 2.20 mL, 5.00 eq.) was added to a mixture of 2-chloro-1,3-di-*tert*-butylimidazolinium chloride (0.80 g, 3.16 mmol, 1.00 eq) and $MeNH_3Cl$ (0.23 g, 3.47 mmol, 1.10 eq) in MeCN (15 mL). The reaction mixture was stirred for two days at 70 °C. After the subsequent work up according to **GP1** the product was isolated as a colorless solid. Yield: 62% (0.59 g, 1.97 mmol).



^{1}H NMR (400.03 MHz, $CDCl_3$): δ = 5.54 (q, $^3J_{HH}$ = 5.2 Hz, 1H, NH), 3.68 (s, 4H, CH_2), 3.08 (d, $^3J_{HH}$ = 5.2 Hz, 3H, NCH_3), 1.46 (s, 18H, $C(CH_3)_3$).

$^{13}C\{^1H\}$ NMR (100.60 MHz, $CDCl_3$): δ = 162.6 (NCN_2), 59.0 ($NC(CH_3)_3$), 44.7 (CH_2), 37.6 (NCH_3), 29.1 (CH_3).

^{11}B NMR (128.38 MHz, $CDCl_3$): δ = -1.0.

$^{11}B\{^1H\}$ NMR (128.38 MHz, $CDCl_3$): δ = -1.0.

^{19}F NMR (376.37 MHz, $CDCl_3$): δ = -152.6.

$^{19}F\{^1H\}$ NMR (376.37 MHz, $CDCl_3$): δ = -152.6.

HRMS (ESI): m/z calculated for $[C_{12}H_{26}N_3]^+$ $(M)^+$ 212.21212, found 212.21129.
Elemental analysis: calculated (%) for $C_{12}H_{26}BF_4N_3$: C 48.18, H 8.76, N 14.05, found C 48.61, H 8.66, N 13.92.
IR (neat): $\tilde{\nu}$ = 1011 (vs), 1058 (vs), 1105 (s), 1180 (s), 1224 (m), 1291 (s), 1377 (s), 1417 (w), 1479 (m), 1543 (m), 1592 (m), 1612 (m), 2988 (w), 3408 (w).

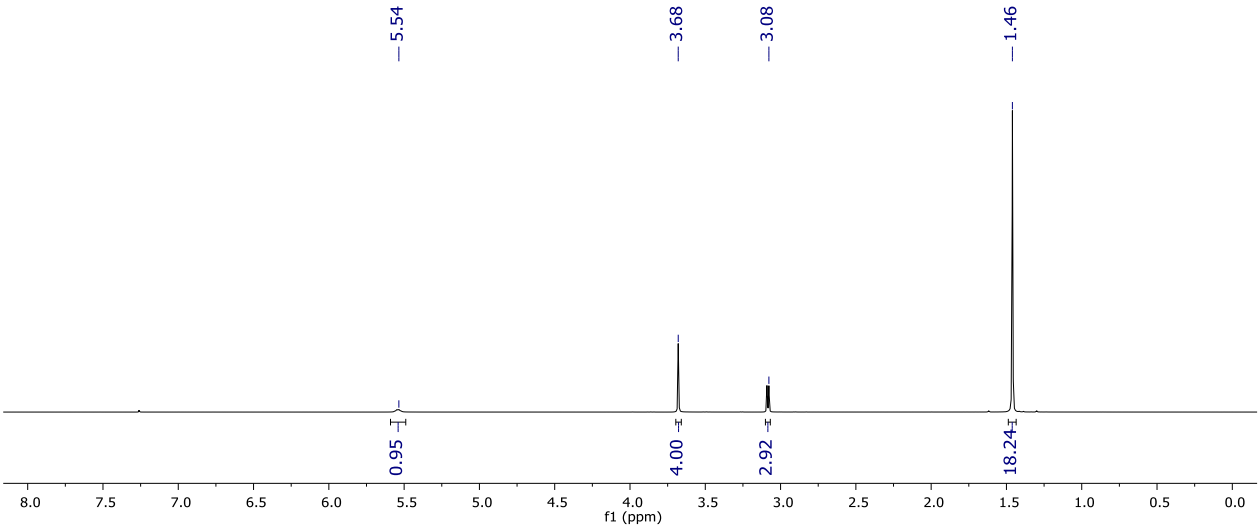


Figure S47: ^{1}H NMR spectrum (in $CDCl_3$, 300 K, 400.03 MHz) of **5**HBF_4.

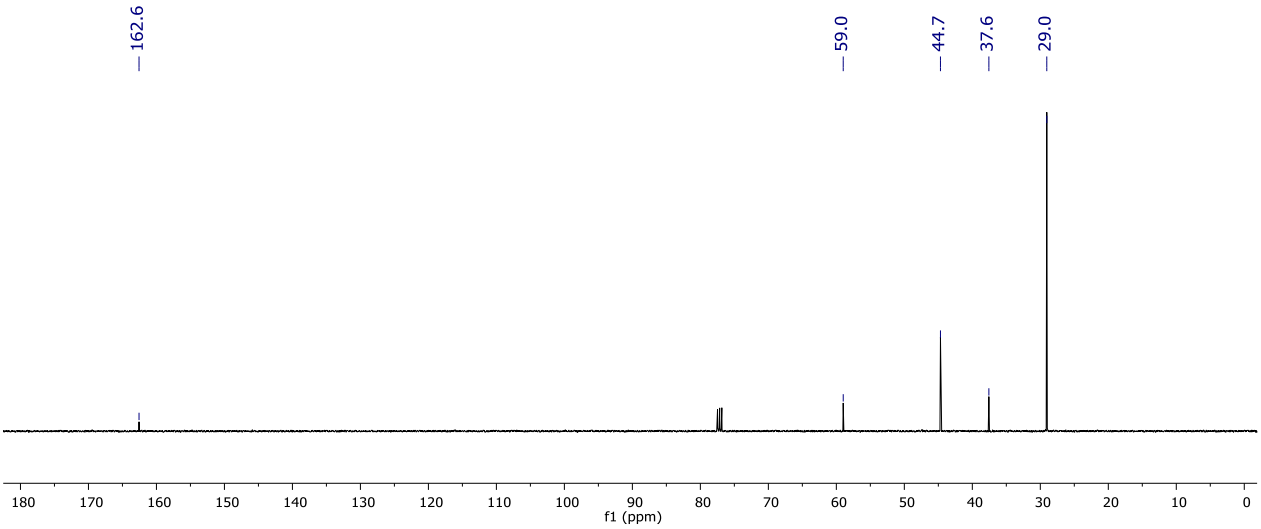


Figure S48: $^{13}C\{^{1}H\}$ NMR spectrum (in $CDCl_3$, 300 K, 100.60 MHz) of **5**HBF_4.

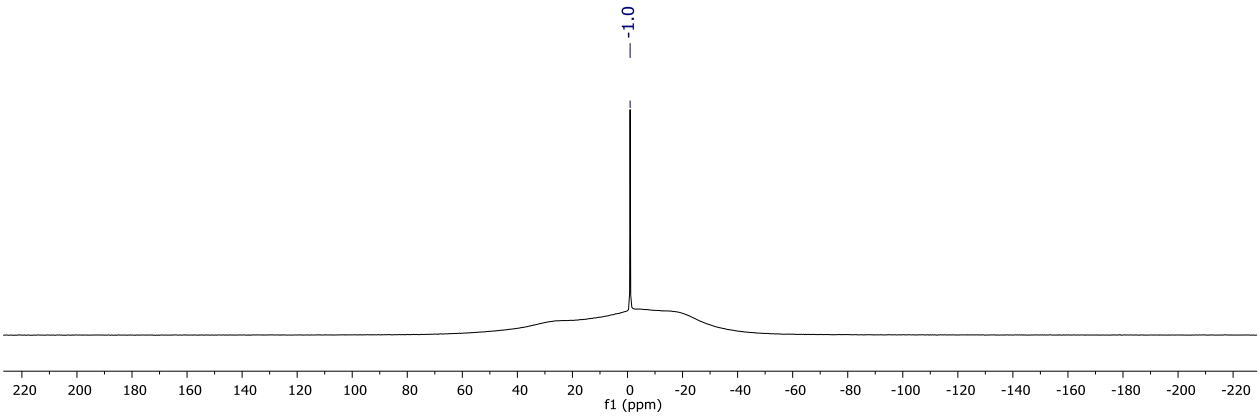


Figure S49: ^{11}B NMR spectrum (in $CDCl_3$, 300 K, 128.38 MHz) of **5**HBF_4.

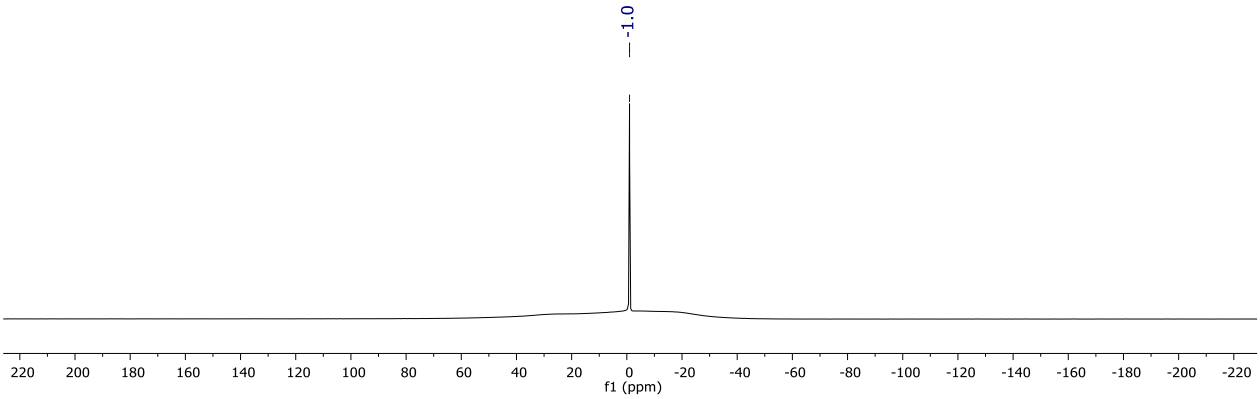


Figure S50: ^{11}B{H} NMR spectrum (in $CDCl_3$, 300 K, 128.38 MHz) of **5**HBF_4.

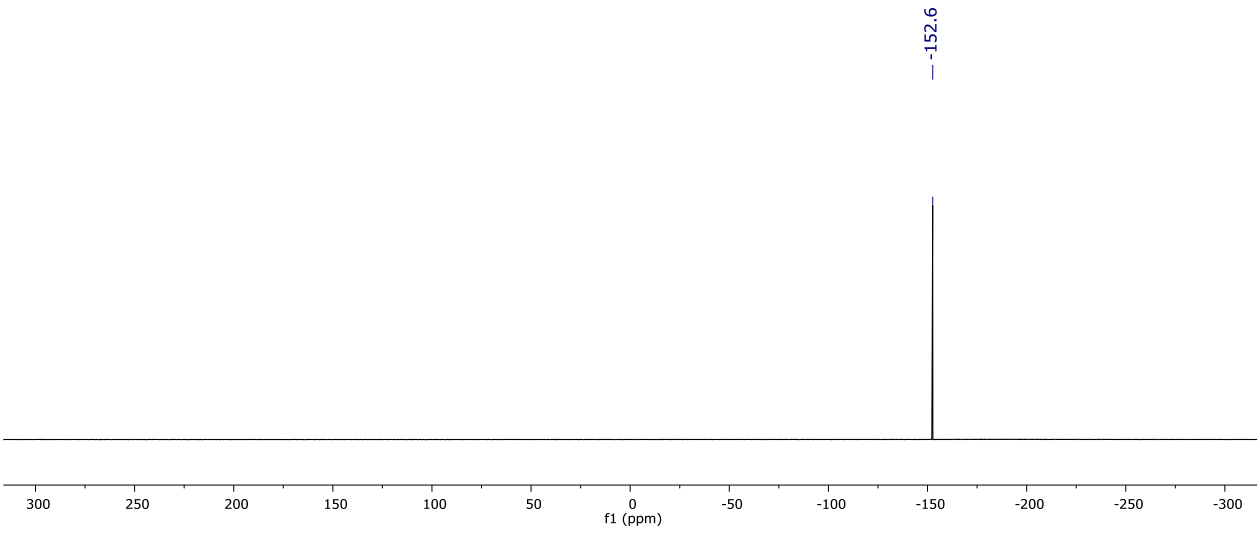


Figure S51: ^{19}F NMR spectrum (in $CDCl_3$, 300 K, 376.37 MHz) of **5**HBF_4.

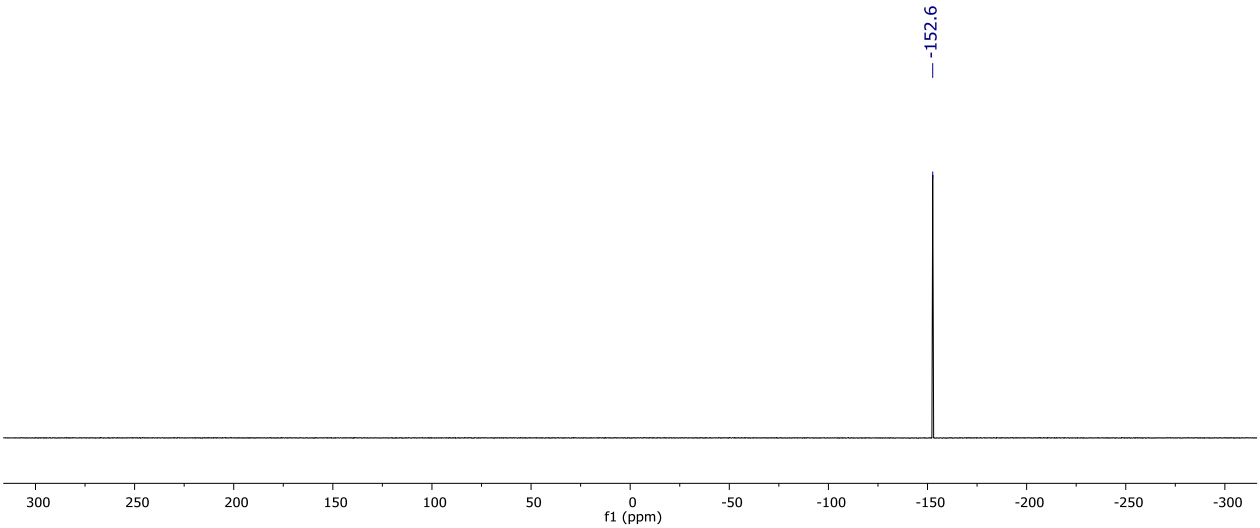
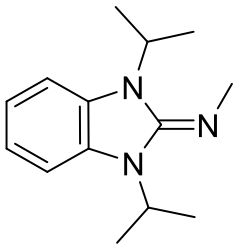


Figure S52: $^{19}F\{H\}$ NMR spectrum (in $CDCl_3$, 300 K, 376.37 MHz) of **5a**HBF_4.

Synthesis of N-heterocyclic imines **2-5**

General procedure GP2: A Schlenk flask was charged with a solution of the N-heterocyclic iminium salt **2**HBF_4-**5**HBF_4 (1.00 eq.) in THF (5.00 mL per 1.00 mmol of **2**HBF_4-**5**HBF_4). A diluted THF solution of KO*t*Bu (0.11 g, 0.98 mmol per 1.00 mmol of **2**HBF_4-**5**HBF_4) was added dropwise and the resulting suspension was stirred at room temperature for 2h. The volatiles were evaporated and the N-heterocyclic imine was extracted twice with *n*-hexane. The solvent was removed under reduced pressure to afford the free N-heterocyclic imine (**2-5**) with a purity of 99% according to NMR analysis.

Compound 2a: Synthesis according to **GP2** starting from **2a**HBF_4 (0.42 g, 1.32 mmol). Yield 96% (0.29 g, 1.26 mmol) as a light yellow oil.



^{1}H NMR (400.13 MHz, MeCN-d_3): δ = 7.00 (m, 2H, aryl-H), 6.83 (m, 2H, aryl-H), 4.90 (hept, $^3J_{HH}$ = 7.0 Hz, 2H, $CH(CH_3)_2$), 3.28 (s, 3H, NCH_3), 1.42 (d, $^3J_{HH}$ = 7.0 Hz, 12H, CH_3).

$^{13}C\{^1H\}$ NMR (100.62 MHz, $CDCl_3$): δ = 147.9 (NCN_2), 132.9 (*ipso*-C), 120.1 (aryl-C), 109.6 (aryl-C), 46.4 ($CH(CH_3)_2$), 35.3 (NCH_3), 20.2 (CH_3).

HRMS (ESI): m/z calculated for $[C_{14}H_{22}N_3]^+$ $(M+H)^+$ 232.18082, found 232.18039.

IR (neat): $\tilde{\nu}$ = 1082 (m), 1111 (m), 1129 (m), 1157 (w), 1169 (w), 1221 (w), 1286 (w), 1302 (m), 1339 (m), 1356 (m), 1378 (w), 1403 (m), 1418 (w), 1460 (s), 1601 (m), 1651 (s), 2864 (w), 2912 (w), 2932 (w), 2971 (w) cm^{-1}.

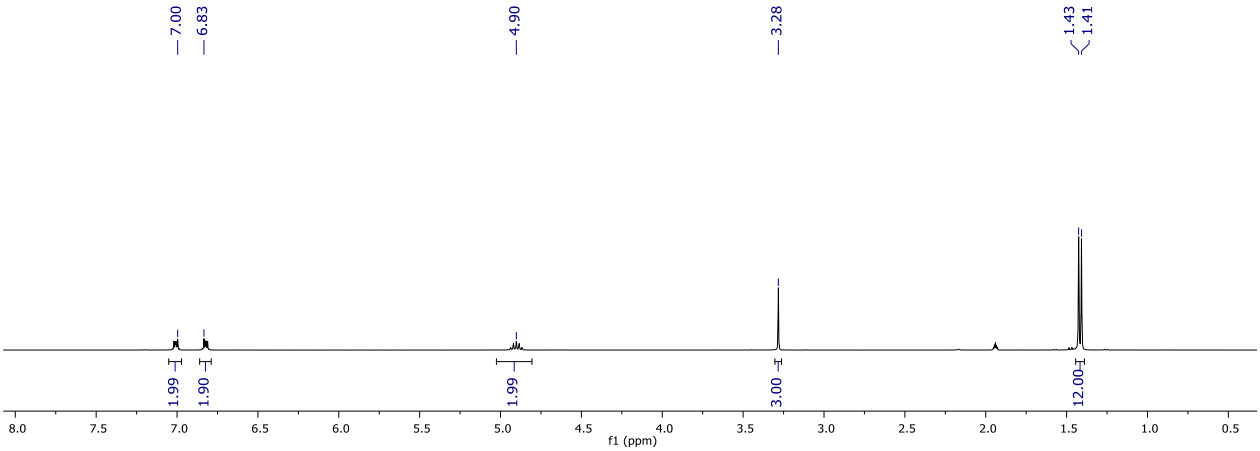


Figure S53: ^{1}H NMR spectrum (in MeCN-d_3, 300 K, 400.13 MHz) of **2a**.

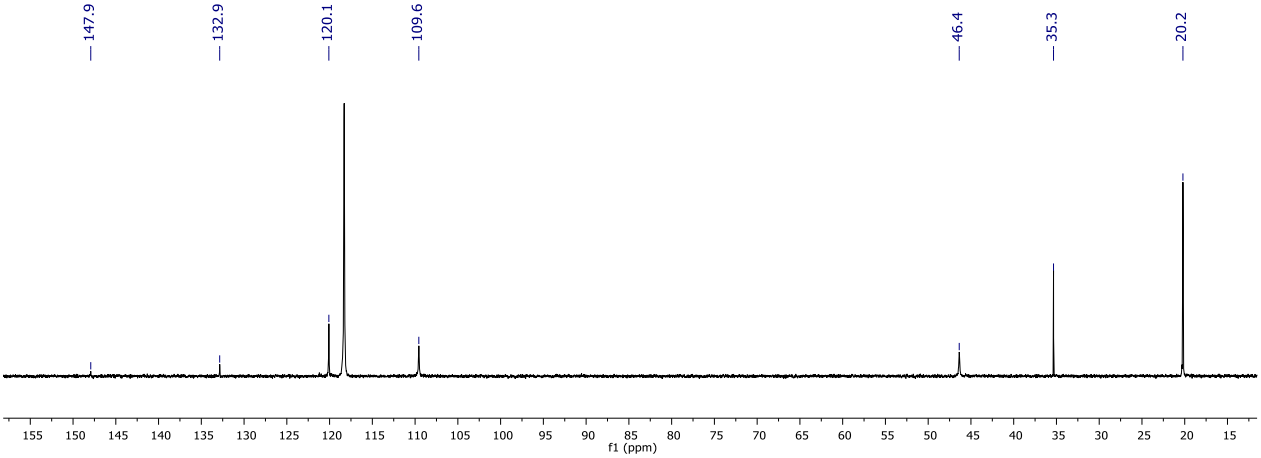
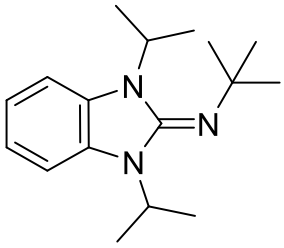


Figure S54: ^{13}C{^{1}H} NMR spectrum (in MeCN-d_3, 300 K, 100.62 MHz) of **2a**.

Compound 2b: Synthesis according to **GP2** starting from **2b**HBF_4 (0.62 g, 1.72 mmol). Yield 94% (0.44 g, 1.62 mmol) as a light yellow oil.



^{1}H NMR (400.13 MHz, MeCN-d_3): δ = 6.99 (m, 2H, aryl-H), 6.82 (m, 2H, aryl-H), 4.81 (hept, $^{3}J_{HH}$ = 7.1 Hz, 2H, $CH(CH_3)_2$), 1.39 (d, $^{3}J_{HH}$ = 7.1 Hz, 12H, CH_3), 1.38 (s, 9H, $C(CH_3)_3$).

^{13}C{^{1}H} NMR (100.62 MHz, MeCN-d_3): δ = 141.2 (NCN_2), 132.9 (*ipso*-C), 119.9 (aryl-C), 109.3 (aryl-C), 51.7 ($NC(CH_3)_3$), 46.6 ($CH(CH_3)_2$), 33.7 ($C(CH_3)_3$), 19.7 (CH_3).

HRMS (ESI): m/z calculated for $[C_{17}H_{28}N_3]^+$ $(M+H)^+$ 274.22777, found 274.22752.

IR (neat): $\tilde{\nu}$ = 1080 (m), 1112 (m), 1133 (m), 1158 (w), 1180 (m), 1287 (w), 1334 (m), 1366 (w), 1415 (w), 1488 (m), 1602 (m), 1646 (s), 2874 (w), 2932 (w), 2966 (w) cm^{-1}.

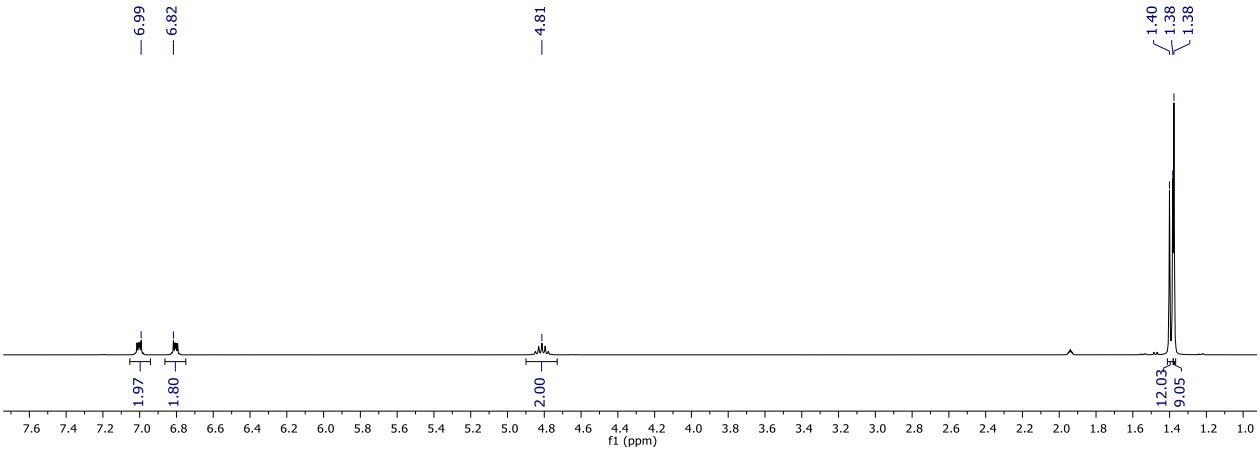


Figure S55: ^{1}H NMR spectrum (in MeCN-d_3, 300 K, 400.13 MHz) of **2b**.

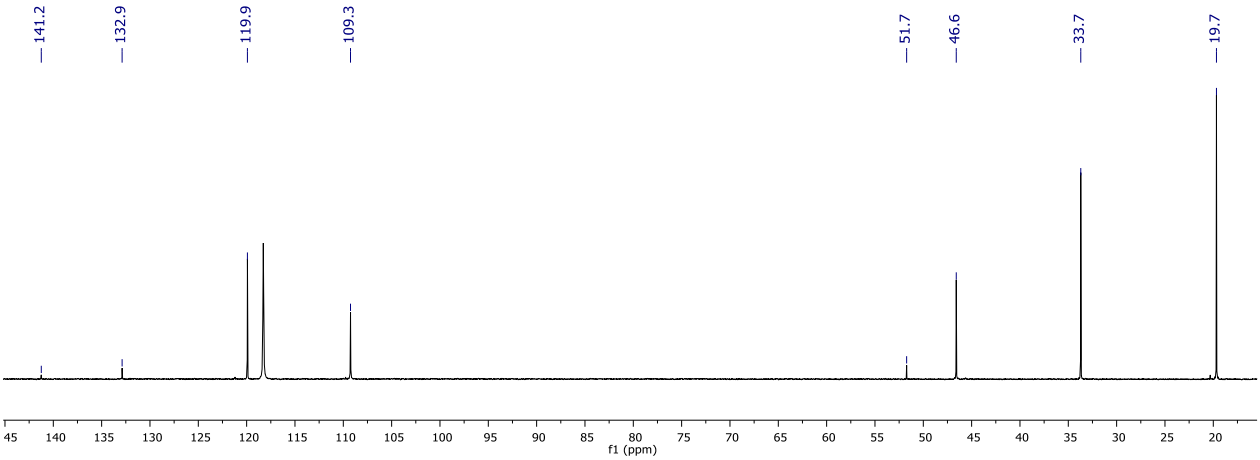
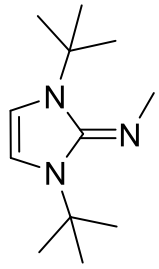


Figure S56: ^{13}C{^{1}H} NMR spectrum (in MeCN-d_3, 300 K, 100.62 MHz) of **2b**.

Compound 3a: Synthesis according to **GP2** starting from **3a**HBF_4 (0.93 g, 3.11 mmol). Yield 94% (0.61 g, 2.91 mmol) as a colorless solid.



^{1}H NMR (400.13 MHz, $CDCl_3$): δ = 6.24 (s, 2H, CH), 3.23 (s, 3H, NCH_3), 1.46 (s, 18H, $C(CH_3)_3$).

^{13}C{^{1}H} NMR (100.62 MHz, $CDCl_3$): δ = 149.0 (NCN_2), 110.0 (CH), 55.5 ($NC(CH_3)_3$), 39.1 (NCH_3), 29.9 ($C(CH_3)_3$).

HRMS (ESI): m/z calculated for $[C_{12}H_{24}N_3]^+$ $(M+H)^+$ 210.19647, found 210.19627.

IR (neat): $\tilde{\nu}$ = 1009 (w), 1083 (w), 1137 (m), 1167 (m), 1203 (vs), 1256 (m), 1282 (w), 1350 (m), 1357 (m), 1366 (m), 1400 (s), 1448 (w), 1479 (w), 1606 (s), 1630 (s), 1672 (w), 2777 (w), 2858 (w), 2957 (w), 2976 (w) cm^{-1}.

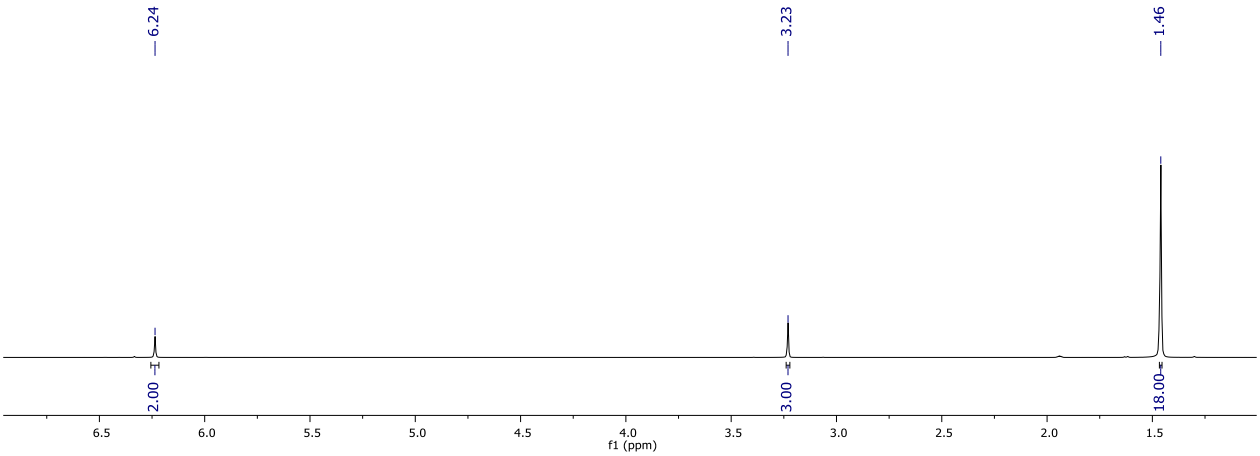


Figure S57: ^{1}H NMR spectrum (in MeCN-d_3, 300 K, 400.13 MHz) of **3a**.

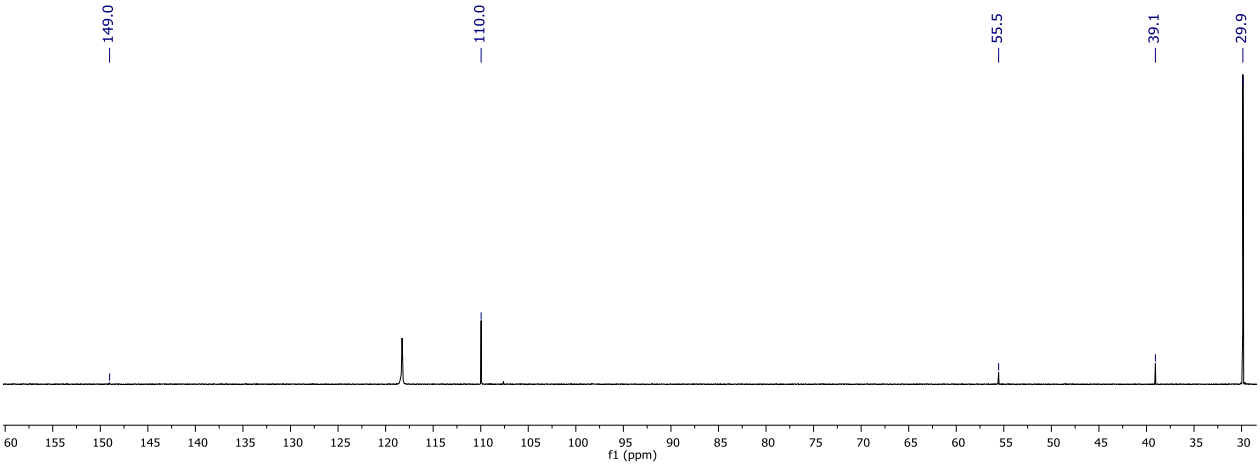
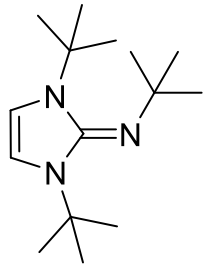


Figure S58: ^{13}C{^{1}H} NMR spectrum (in MeCN-d_3, 300 K, 100.62 MHz) of **3a**.

Compound 3b: Synthesis according to **GP2** starting from **3b**HBF_4 (1.40 g, 4.13 mmol). Yield 95% (0.99 g, 3.94 mmol) as a light yellow oil.



^{1}H NMR (400.03 MHz, MeCN-d_3): δ = 6.25 (s, 2H, CH), 1.42 (s, 18H, $C(CH_3)_3$), 1.34 (s, 9H, CH_3).

^{13}C{^{1}H} NMR (100.60 MHz, MeCN-d_3): δ = 145.9 (NCN_2), 112.9 (CH), 56.3 ($2xNC(CH_3)_3$), 55.4 ($NC(CH_3)_3$), 33.3 ($6xCH_3$), 29.4 ($3xCH_3$).

HRMS (ESI): m/z calculated for $[C_{15}H_{30}N_3]^+$ $(M)^+$ 252.24342, found 252.24258.

IR (neat): $\tilde{\nu}$ = 1021 (w), 1058 (w), 1101 (m), 1185 (vs), 1245 (m), 1291 (s), 1361 (s), 1376 (m), 1391 (m), 1453 (m), 1585 (m), 1645 (s), 2925 (m), 2971 (s), 3118 (w) cm^{-1}.

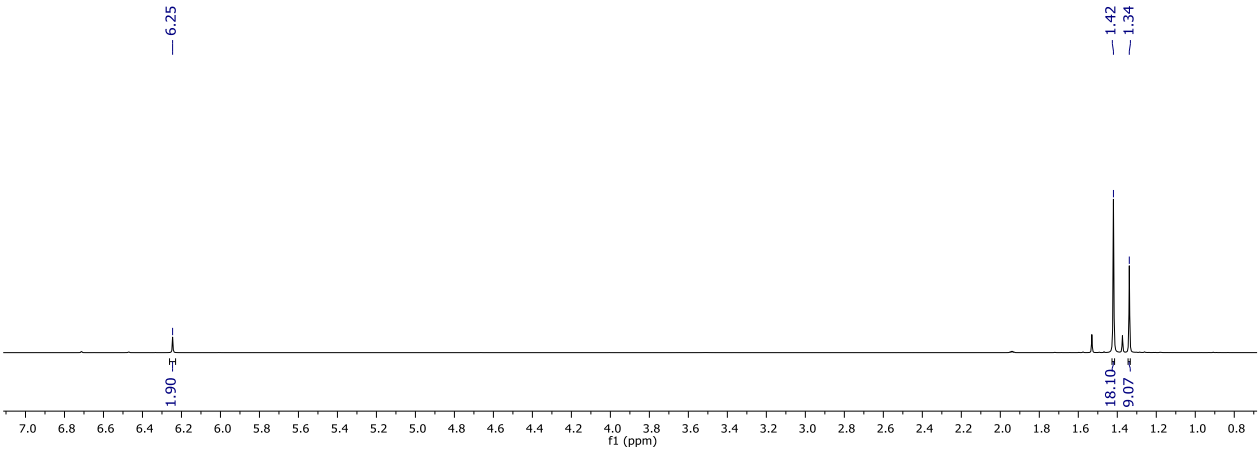


Figure S59: ^{1}H NMR spectrum (in MeCN-d_3, 300 K, 400.03 MHz) of **3b**.

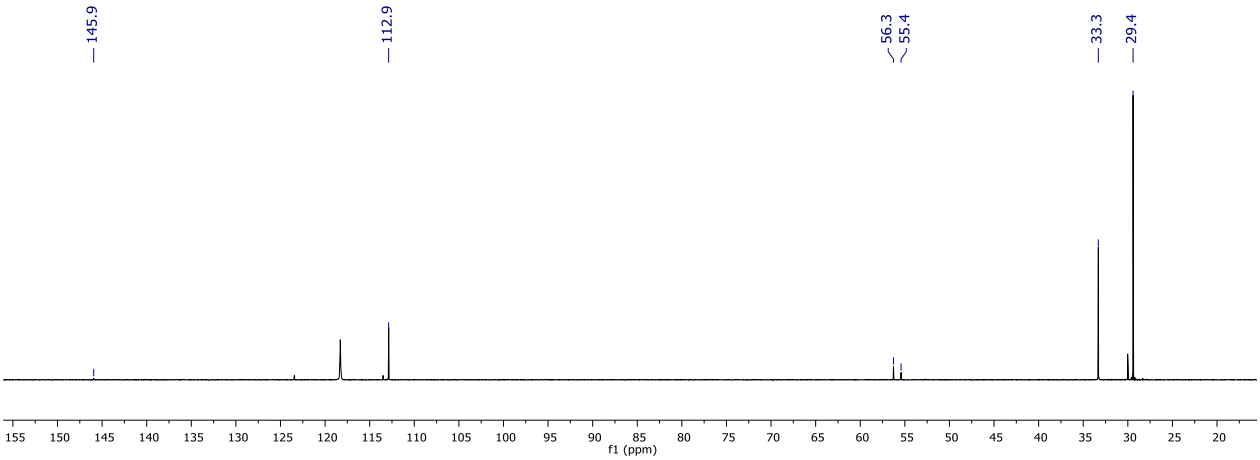
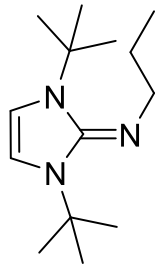


Figure S60: ^{13}C{^{1}H} NMR spectrum (in MeCN-d_3, 300 K, 100.60 MHz) of **3b**.

Compound 3c: Synthesis according to **GP2** starting from **3c**HBF_4 (1.44 g, 4.43 mmol). Yield 94% (0.99 g, 4.16 mmol) as a light yellow oil.



^{1}H NMR (400.03 MHz, MeCN-d_3): δ = 6.22 (s, 2H, CH), 3.42 (t, $^{3}J_{HH}$ = 6.6 Hz, 2H, NCH_2), 1.54 (hept, $^{3}J_{HH}$ = 7.1 Hz, 2H, CH_2), 1.47 (s, 18H, $C(CH_3)_3$), 0.97 (t, $^{3}J_{HH}$ = 7.3 Hz, 3H, CH_3).

^{13}C{^{1}H} NMR (100.60 MHz, MeCN-d_3): δ = 146.8 (NCN_2), 109.6 (CH), 55.5 ($NC(CH_3)_3$), 54.2 (NCH_2CH_2), 29.9 ($C(CH_3)_3$), 28.3 (CH_2), 12.6 (CH_3).

^{13}C{^{1}H}-DEPT135° NMR (100.59 MHz, MeCN-d_3): δ = 109.7 (CH), 54.3 (NCH_2CH_2), 29.9 ($C(CH_3)_3$), 28.3 (CH_2), 12.7 (CH_3).

HRMS (EI): m/z calculated for $[C_{14}H_{28}N_3]^+$ $(M+H)^+$ 238.22777, found 238.22747.

IR (neat): $\tilde{\nu}$ = 1144 (w), 1166 (w), 1221 (s), 1314 (w), 1357 (m), 1401 (m), 1451 (w), 1604 (m), 1637 (s), 2818 (w), 2870 (w), 2919 (m), 2957 (m) cm^{-1}.

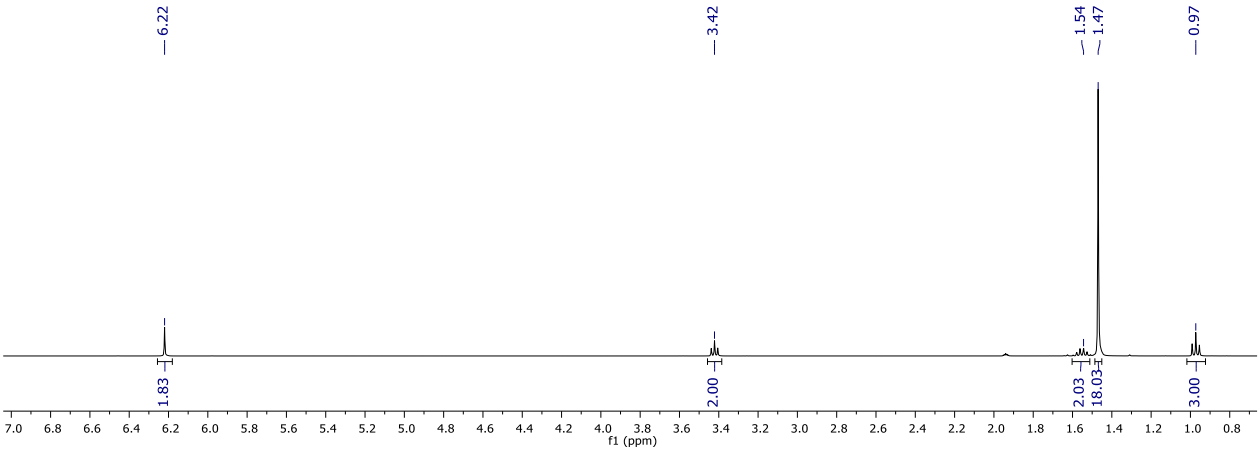


Figure S61: ^{1}H NMR spectrum (in MeCN-d_3, 300 K, 400.03 MHz) of **3c**.

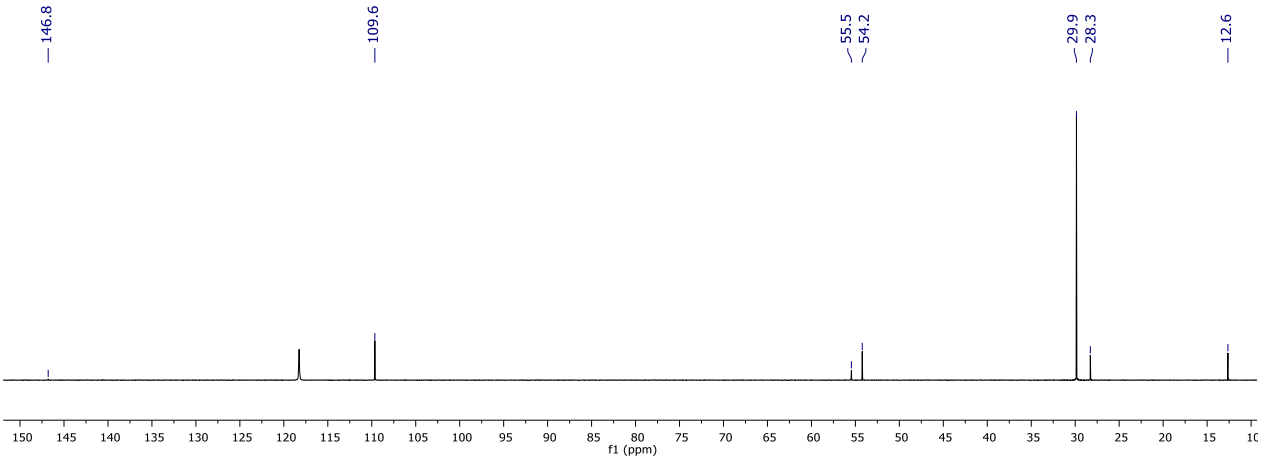


Figure S62: ^{13}C{^{1}H} NMR spectrum (in MeCN-d_3, 300 K, 100.60 MHz) of **3c**.

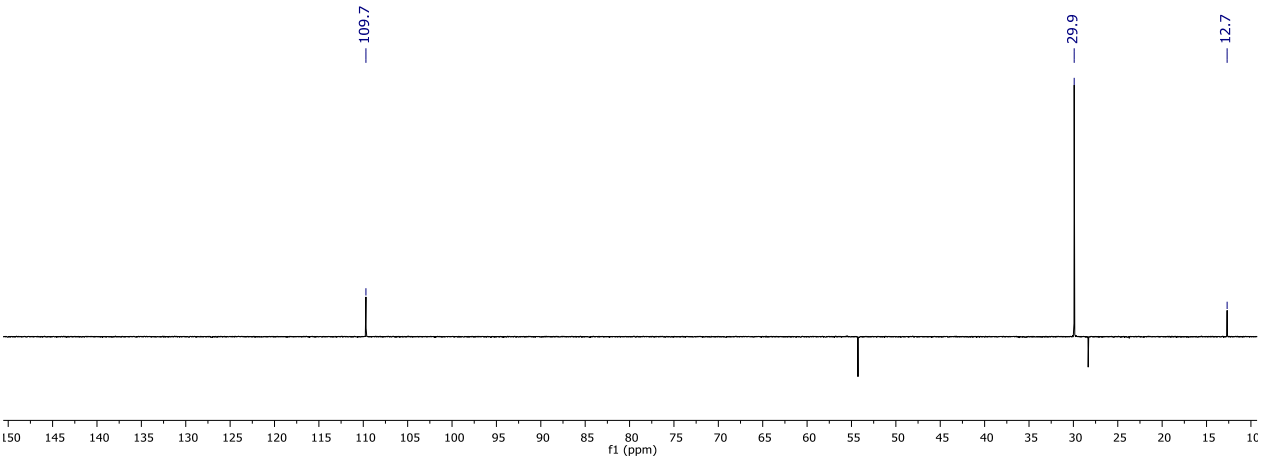
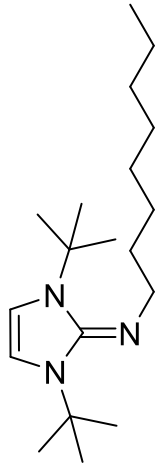


Figure S63: ^{13}C{^{1}H}-DEPT135° NMR spectrum (in MeCN-d_3, 300 K, 100.59 MHz) of **3c**.

Compound 3d: Synthesis according to **GP2** starting from **3d**HBF_4 (1.26 g, 3.19 mmol). Yield 87% (0.85 g, 2.76 mmol) as a colorless oil.



^{1}H NMR (400.13 MHz, C_6D_6): δ = 6.01 (s, 2H, CH), 3.70 (t, $^3J_{HH}$ = 6.6 Hz, 2H, NCH_2), 1.88 (m, 2H, CH_2), 1.66 (m, 2H, CH_2), 1.47 (m, 2H, CH_2), 1.44 (s, 18H, $C(CH_3)_3$), 1.38 (m, 2H, CH_2), 1.29 (m, 4H, 2xCH_2), 0.89 (m, 3H, CH_3).

^{13}C{^{1}H} NMR (100.62 MHz, C_6D_6): δ = 145.9 (NCN_2), 108.8 (CH), 54.7 ($NC(CH_3)_3$), 52.0 (NCH_2), 35.2 (CH_2), 32.4 (CH_2), 30.4 (CH_2), 30.0 (CH_2), 29.8 ($C(CH_3)_3$), 28.3 (CH_2), 23.1 (CH_2), 14.4 (CH_3).

HRMS (EI): m/z calculated for $[C_{19}H_{38}N_3]^+$ $(M+H)^+$ 308.30602, found 308.30514.

IR (neat): $\tilde{\nu}$ = 1143 (w), 1166 (w), 1220 (s), 1313 (w), 1359 (m), 1401 (m), 1452 (m), 1604 (m), 1638 (vs), 2853 (m), 2921 (m), 2958 (m) cm^{-1}.

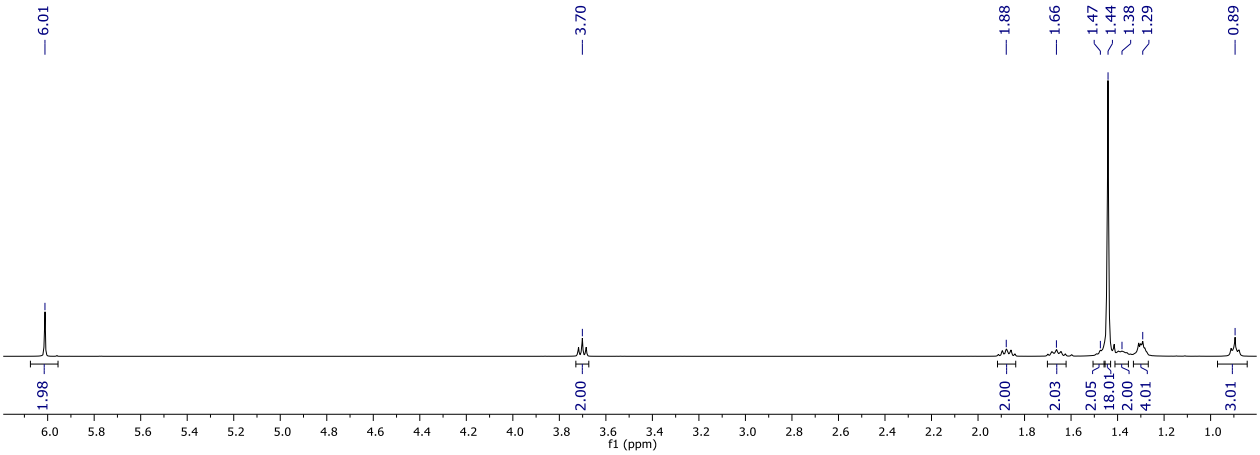


Figure S64: ^{1}H NMR spectrum (in C_6D_6, 300 K, 400.13 MHz) of **3d**.

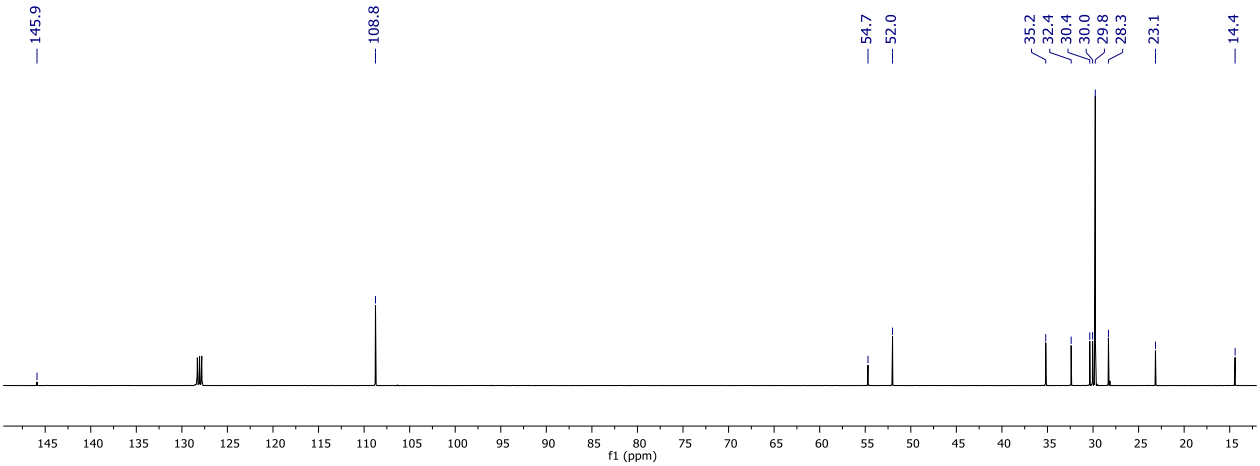
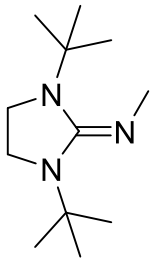


Figure S65: ^{13}C{^{1}H} NMR spectrum (in C_6D_6, 300 K, 100.62 MHz) of **3d**.

Compound 5a: Synthesis according to **GP2** starting from **5a**HBF_4 (0.25 g, 0.84 mmol). Yield: 82% (0.15 g, 0.69 mmol) as a colorless oil.



^{1}H NMR (400.13 MHz, MeCN-d_3): δ = 3.08 (s, 4H, CH_2), 2.97 (s, 3H, NCH_3), 1.24 (s, 18H, $C(CH_3)_3$).

^{13}C{^{1}H} NMR (100.62 MHz, MeCN-d_3): δ = 157.4 (NCN_2), 55.6 ($NC(CH_3)_3$), 44.0 (CH_2), 40.4 (NCH_3), 27.9 (CH_3).

HRMS (EI): m/z calculated for $[C_{12}H_{26}N_3]^+$ $(M+H)^+$ 212.21212, found 212.21217.

IR (neat): $\tilde{\nu}$ = 1047 (m), 1188 (s), 1218 (m), 1239 (s), 1263 (m), 1360 (s), 1391 (s), 1456 (m), 1476 (m), 1657 (vs, ν(C=N)), 2765 (w), 2862 (s), 2909 (s), 2969 (s) cm^{-1}.

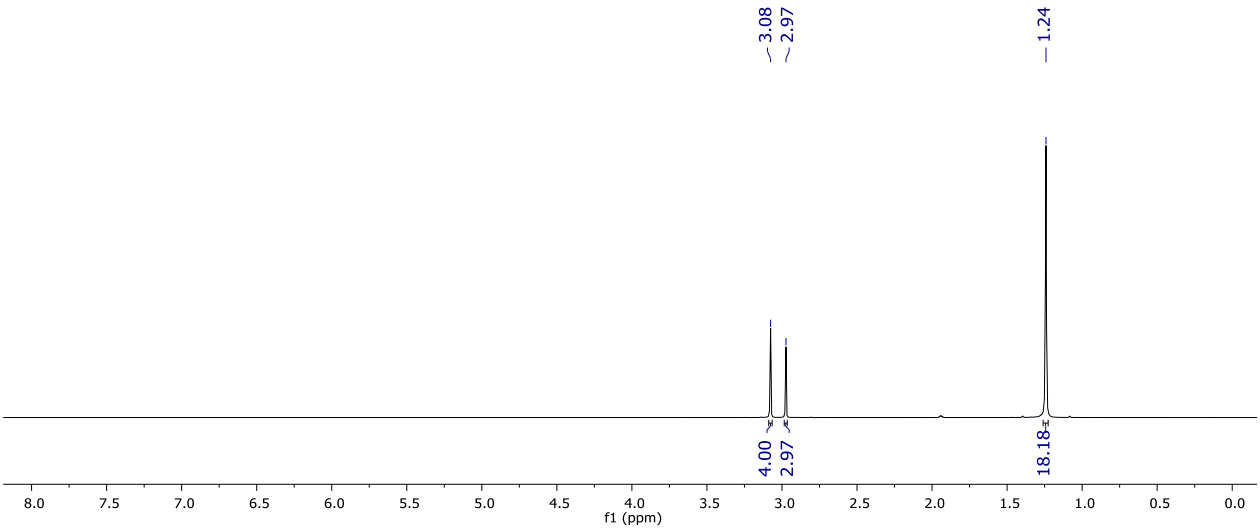


Figure S66: ^{1}H NMR spectrum (in MeCN-d_3, 300 K, 400.13 MHz) of **5a**.

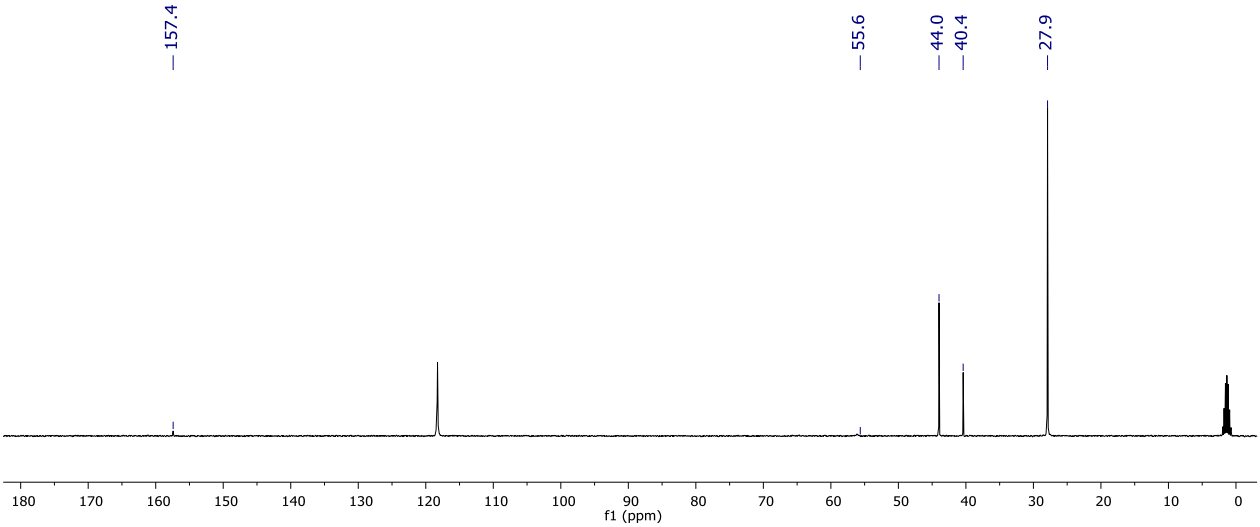
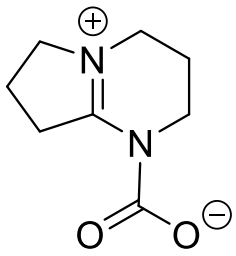


Figure S67: ^{13}C{^{1}H} NMR spectrum (in MeCN-d_3, 300 K, 100.62 MHz) of **5a**.

Synthesis of **1** and of NHI–CO_2 adducts **6a-d** and **7a-d**

General procedure GP3: Pressurizing a pentane solution of the N-heterocyclic imine with 2 bar carbon dioxide pressure resulted in the precipitation of the NHI–CO_2 adduct. The white precipitate was separated by filtration and was dried under argon atmosphere.

Compound 1: Synthesis according to **GP3** starting from DBN (0.10 g, 0.81 mmol). Yield 100% (0.14 g, 0.81 mmol) as a white solid. For the NMR analysis of DBN–CO_2 (**1**), DBN (0.05 g, 0.40 mmol) was dissolved in MeCN-d_3 and the NMR-tube was pressurized with two bar ^{13}C-labeled carbon dioxide pressure.



^{1}H NMR (400.13 MHz, MeCN-d_3): δ = 3.27 (t, $^3J_{HH}$ = 7.0 Hz, 2H, CH_2), 3.16 (t, $^3J_{HH}$ = 6.1 Hz, 2H, CH_2), 2.49 (t, $^3J_{HH}$ = 7.9 Hz, 2H, CH_2), 1.88 (p, $^3J_{HH}$ = 7.3 Hz, 2H, CH_2), 1.73 (p, $^3J_{HH}$ = 5.9 Hz, 2H, CH_2).

^{13}C{^{1}H} NMR (100.62 MHz, MeCN-d_3): δ = 161.9 (CCN_2), 131.3 (NCO_2), 52.5 (CH_2CN), 44.3 (CH_2CN), 44.0 (CH_2CN), 32.3 (CH_2C_qC), 21.5 (CH_2), 20.3 (CH_2).

^{15}N NMR (40.55 MHz, MeCN-d_3): δ = 184.0 (NCO_2), 98.9 (NC_3).

IR (neat): $\tilde{\nu}$ = 1049 (m), 1077 (m), 1133 (m), 1192 (s), 1205 (s), 1222 (m), 1279 (s), 1312 (m), 1360 (m), 1413 (m), 1456 (w), 1510 (m), 1620 (s), 1651 (s), 1727 (m, ν(C=O)), 2818 (w), 2841 (m), 2885 (w), 2926 (m) cm^{-1}.

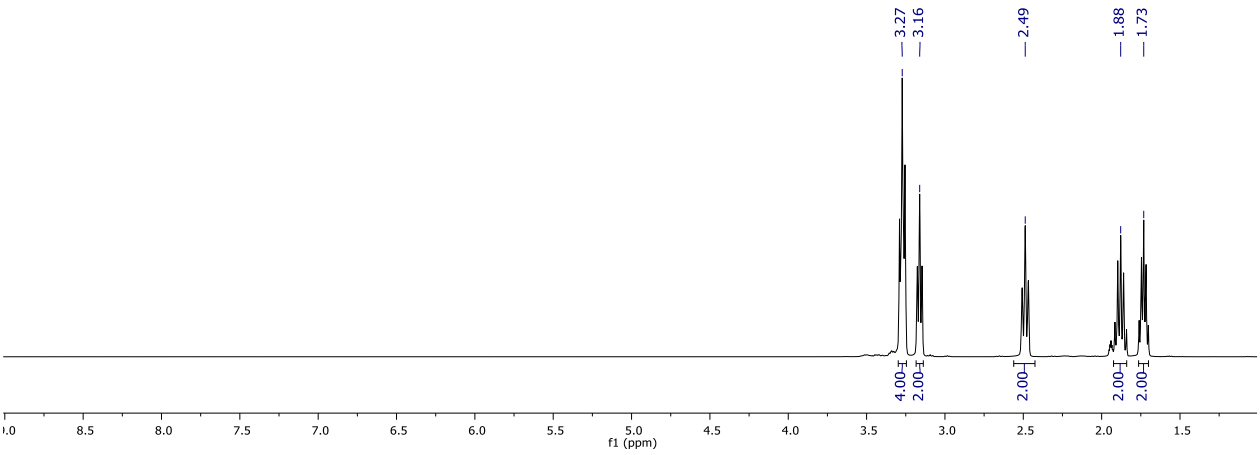


Figure S68: ^{1}H NMR spectrum (in MeCN-d_3, 300 K, 400.13 MHz) of **1**.

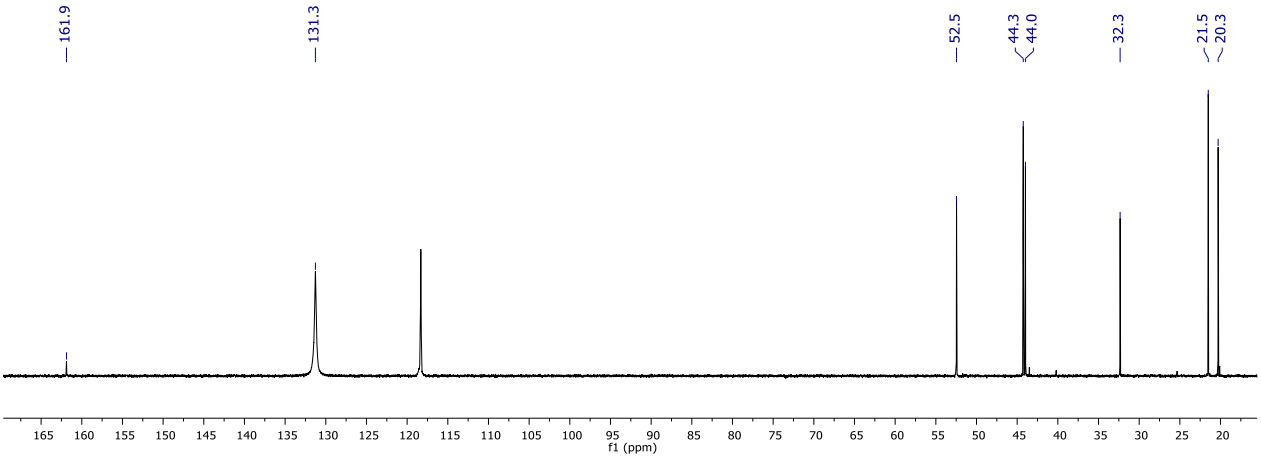


Figure S69: $^{13}C\{^{1}H\}$ NMR spectrum (in MeCN-d_3, 300 K, 100.62 MHz) of **1** prepared using ^{13}C-enriched carbon dioxide gas.

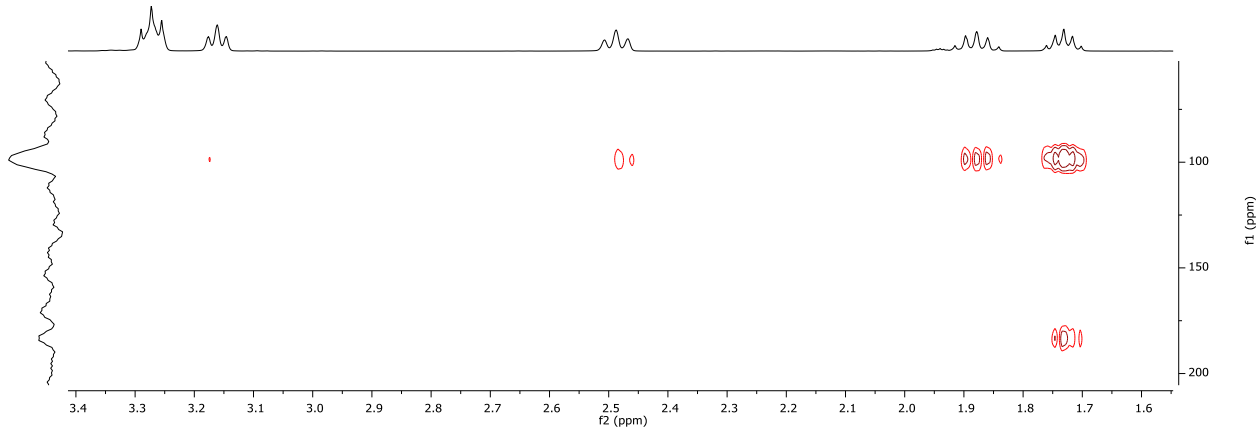
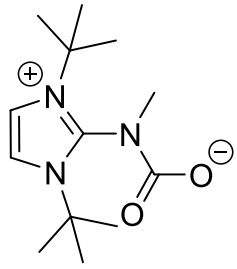


Figure S70: ^{1}H-^{15}N-HMBC NMR spectrum (in MeCN-d_3, 300 K, 400.13, 40.55 MHz) of **1**.

Compound 6a: Synthesis according to **GP3** starting from **3a** (0.10 g, 0.48 mmol). Yield 100% (0.12 g, 0.48 mmol) as a white solid.



^{1}H NMR (400.13 MHz, MeCN-d_3): δ = 7.38 (s, 2H, CH), 2.91 (s, 3H, NCH_3), 1.64 (s, 18H, $C(CH_3)_3$).

$^{13}C\{^{1}H\}$ NMR (100.62 MHz, MeCN-d_3): δ = 157.8 (NCO_2), 144.2 (N_2CN) 118.8 (CH), 62.8 ($NC(CH_3)_3$), 38.6 (CH_3), 30.0 ($C(CH_3)_3$).

^{15}N NMR (40.55 MHz, MeCN-d_3): δ = 197.3 (NC_3), 72.4 (NCO_2).

HRMS (ESI): m/z calculated for $[C_{13}H_{23}N_3O_2Na]^+$ $(M+Na)^+$ 276.16825, found 276.16818.

IR (neat): $\tilde{\nu}$ = 1084 (w), 1157 (m), 1179 (m), 1234 (m), 1256 (s), 1276 (s), 1338 (m), 1372 (w), 1413 (w), 1449 (m), 1484 (m), 1575 (m), 1666 (vs,ν(C=O)), 2946 (m), 2970 (m), 3015 (w), 3067 (m), 3093 (m) cm^{-1}.

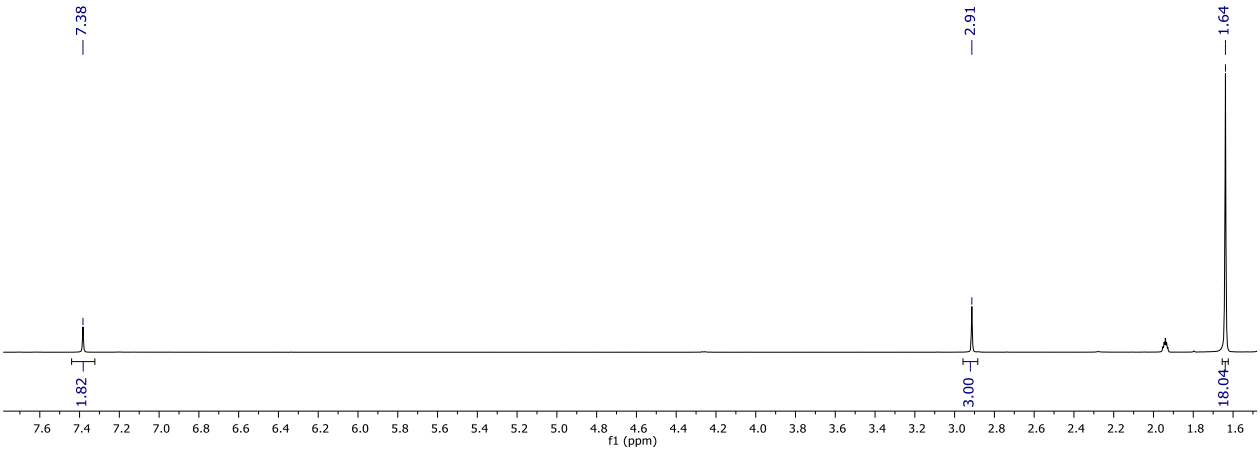


Figure S71: ^{1}H NMR spectrum (in MeCN-d_3, 300 K, 400.13 MHz) of **6a**.

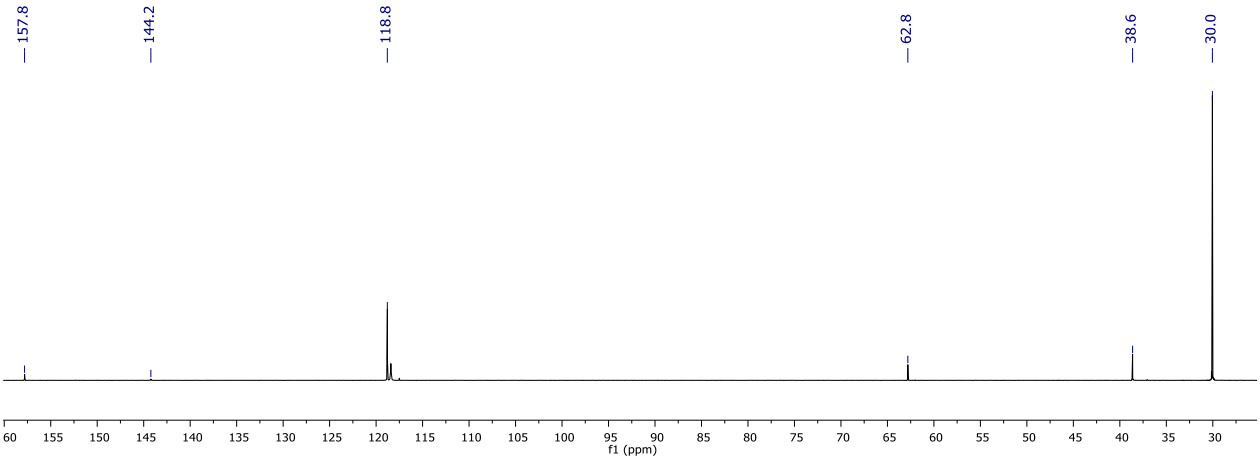


Figure S72: ^{13}C{^{1}H} NMR spectrum (in MeCN-d_3, 300 K, 100.62 MHz) of **6a**.

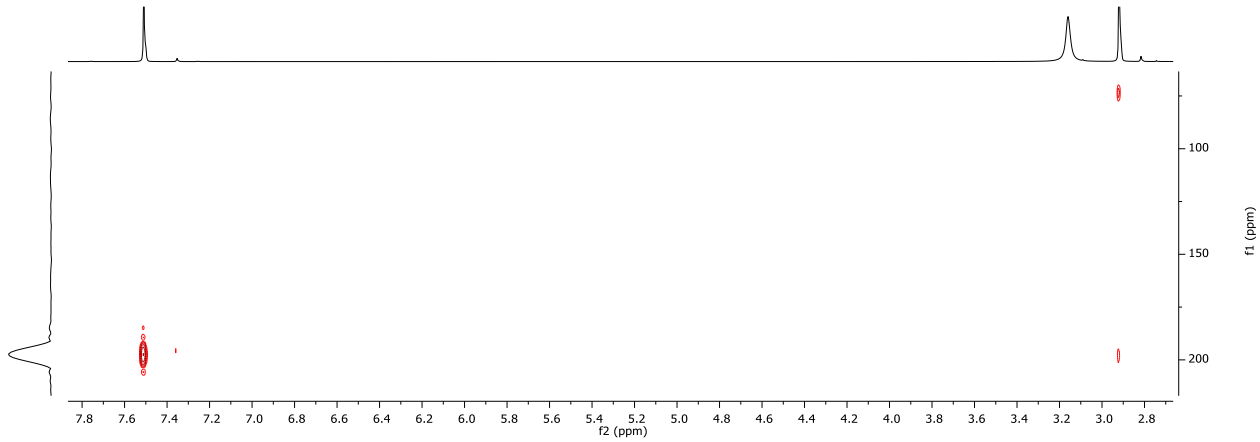
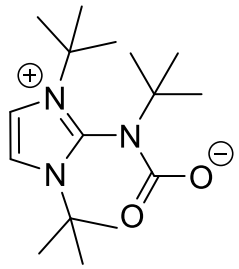


Figure S73: ^{1}H-^{15}N-HMBC NMR spectrum (in MeCN-d_3, 300 K, 400.13, 40.55 MHz) of **6a**.

Compound 6b: Synthesis according to **GP3** starting from **5a** (0.10 g, 0.40 mmol). Yield 100% (0.12 g, 0.40 mmol) as a white solid. For the NMR analysis of **6b**, **3b** (0.05 g, 0.40 mmol) was dissolved in MeCN-d_3 and the NMR-tube was pressurized with two bar ^{13}C-labeled carbon dioxide pressure.



^{1}H NMR (400.03 MHz, MeCN-d_3): δ = 7.49 (s, 2H, CH), 1.73 (s, 18H, $C(CH_3)_3$), 1.44 (s, 9H, NCH_3).

^{13}C{^{1}H} NMR (100.60 MHz, MeCN-d_3): δ = 156.9 (NCO_2), 146.3 (N_2CN) 119.2 (CH), 64.3 (2x$NC(CH_3)_3$), 58.9 ($NC(CH_3)_3$), 30.6 (6xCH_3), 29.5 (3xCH_3).

HRMS (ESI): m/z calculated for $[C_{15}H_{30}N_3]^+$ $(M\text{-}CO_2+H)^+$ 252.24342, found 252.24322.

IR (neat): $\tilde{\nu}$ = 1000 (w), 1128 (m), 1186 (vs), 1226 (s), 1254 (s), 1303 (s), 1344 (m), 1371 (vs), 1386 (s), 1455 (m), 1475 (m), 1537 (m), 1582 (m), 1614 (s), 1627 (vs), 1654 (s,ν(C=O)), 2874 (m), 2974 (vs), 3100 (m), 3162 (w) cm^{-1}.

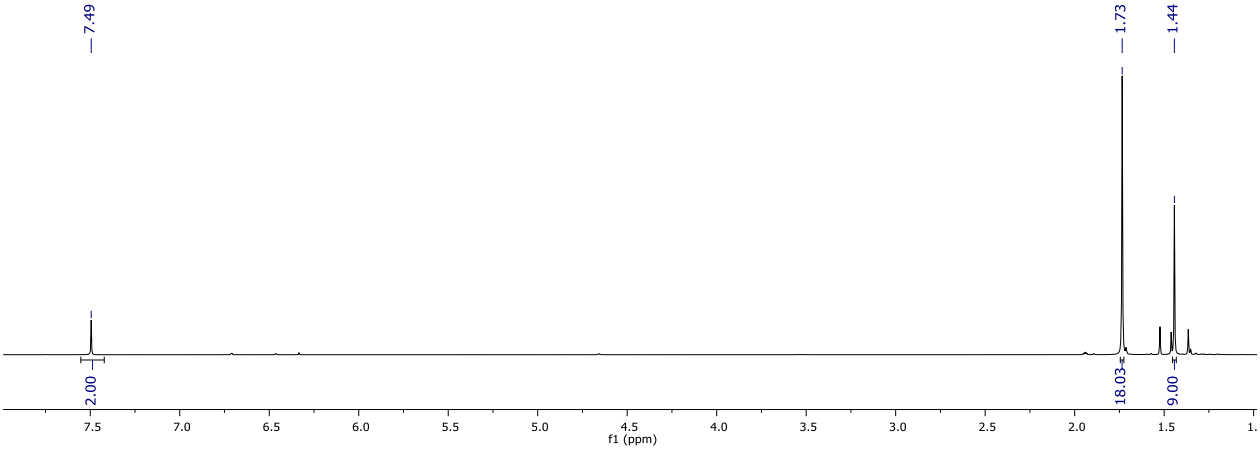


Figure S74: ^{1}H NMR spectrum (in MeCN-d_3, 300 K, 400.03 MHz) of **6b**.

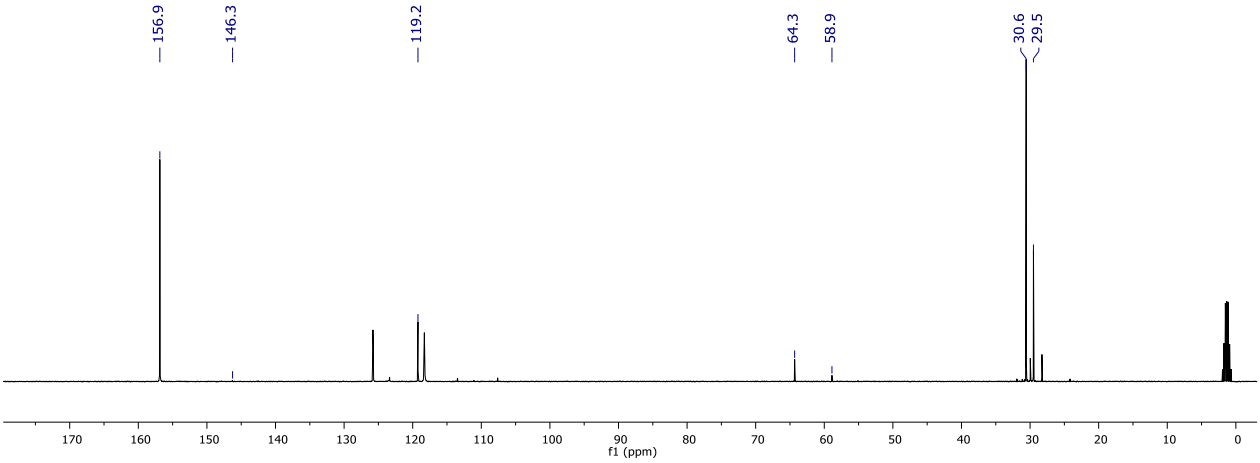
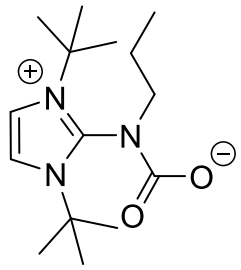


Figure S75: ^{13}C{^{1}H} NMR spectrum (in MeCN-d_3, 300 K, 100.60 MHz) of **6b** prepared using ^{13}C-enriched carbon dioxide gas.

Compound 6c: Synthesis according to **GP3** starting from **3c** (0.10 g, 0.42 mmol). Yield 100% (0.12 g, 0.42 mmol) as a white solid.



^{1}H NMR (400.13 MHz, $CDCl_3$): δ = 7.48 (s, 2H, CH), 3.25 (m, 2H, CH_2), 1.63 (s, 18H, $C(CH_3)_3$), 1.32 (m, 2H, CH_2), 0.88 (t, $^{3}J_{HH}$ = 7.3 Hz, 3H, CH_3).

^{13}C{^{1}H} NMR (100.62 MHz, $CDCl_3$): δ = 157.0 (NCO_2), 144.3 (NCN_2), 118.9 (CH), 63.1 ($NC(CH_3)_3$), 53.0 (NCH_2CH_2), 30.1 ($C(CH_3)_3$), 21.4 (CH_2), 12.0 (CH_3).

HRMS (EI): m/z calculated for $[C_{14}H_{28}N_3]^+$ $(M\text{-}CO_2+H)^+$ 238.22777, found 238.22820.

IR (neat): $\tilde{\nu}$ = 1087 (m), 1146 (m), 1168 (m), 1192 (s), 1223 (s), 1256 (s), 1276 (s), 1304 (m), 1337 (m), 1358 (m), 1372 (m), 1401 (m), 1450 (m), 1582 (m), 1605 (m), 1638 (vs), 1665 (vs, ν(C=O)), 2873 (w), 2928 (m), 2960 (m) cm^{-1}.

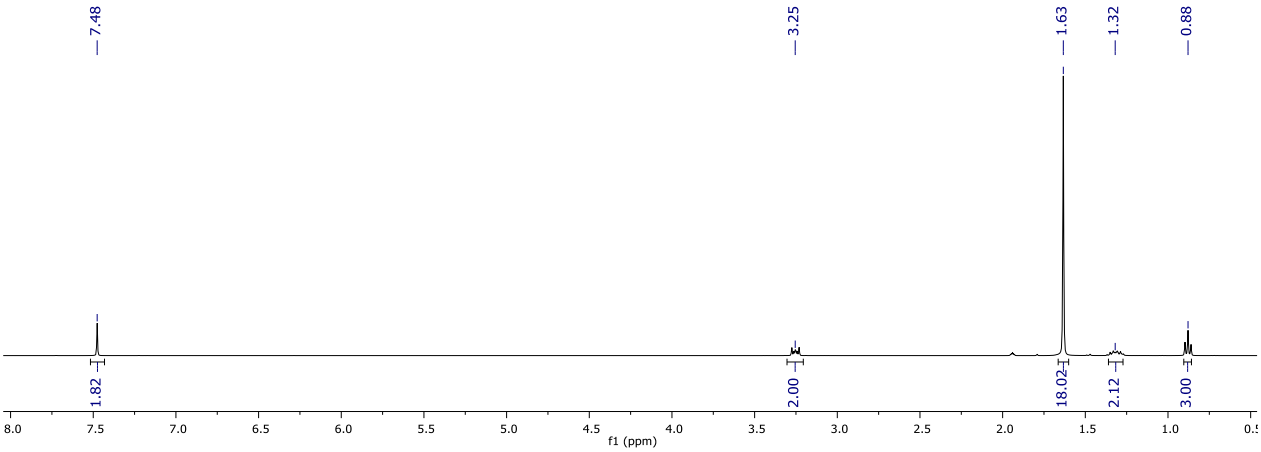


Figure S76: ^{1}H NMR spectrum (in MeCN-d_3, 300 K, 400.13 MHz) of **6c**.

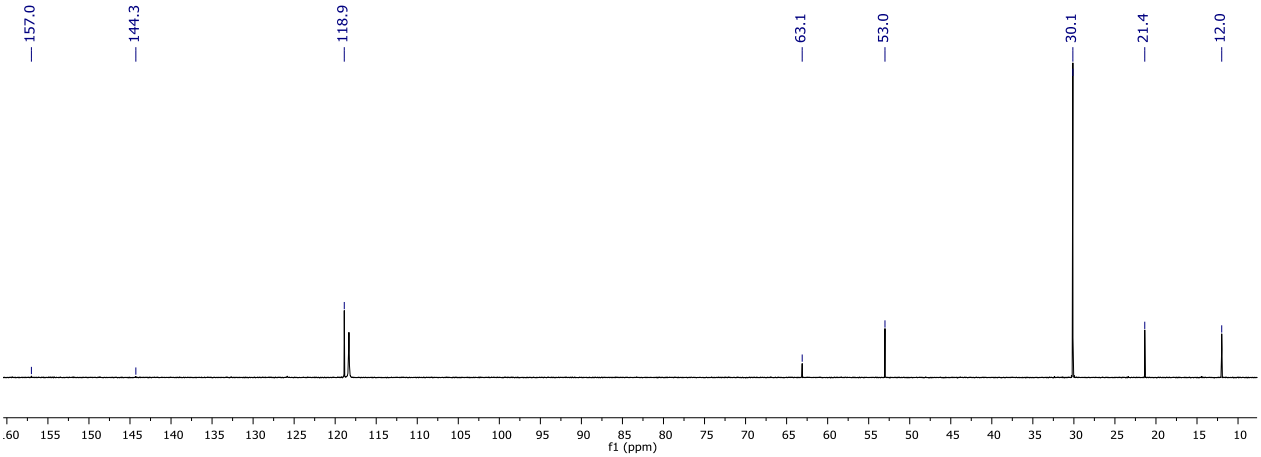
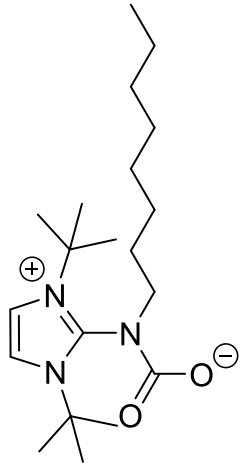


Figure S77: ^{13}C{^{1}H} NMR spectrum (in MeCN-d_3, 300 K, 100.62 MHz) of **6c**.

Compound 6d: Synthesis according to **GP3** starting from **3d** (0.10 g, 0.33 mmol). Yield 100% (0.11 g, 0.33 mmol) as a white solid.



^{1}H NMR (400.13 MHz, C_6D_6): δ = 8.31 (br, 2H, CH), 3.61 (m, 2H, NCH_2), 1.57 (s, 18H, $C(CH_3)_3$), 1.34 (m, 2H, CH_2), 1.22 (m, 2H, CH_2), 1.17 (br, 8H, 4xCH_2), 0.86 (t, $^{3}J_{HH}$ = 7.0 Hz, 3H, CH_3).

^{13}C{^{1}H} NMR (100.62 MHz, C_6D_6): δ = 157.1 (NCO_2) 143.1 (NCN_2), 120.5 (CH), 61.7 ($NC(CH_3)_3$), 51.2 (NCH_2), 32.1 (CH_2), 30.1 (CH_2), 30.1 ($C(CH_3)_3$), 29.7 (CH_2), 29.7 (CH_2), 28.0 (CH_2), 23.0 (CH_2), 14.3 (CH_3).

HRMS (EI): m/z calculated for $[C_{19}H_{38}N_3]^+$ $(M\text{-}CO_2+H)^+$ 308.30602, found 308.30514.

IR (neat): $\tilde{\nu}$ = 1098 (m), 1146 (m), 1192 (s), 1229 (m), 1257 (s), 1278 (s), 1336 (m), 1360 (w), 1374 (m), 1402 (w), 1449 (m), 1582 (m), 1605 (w), 1641 (s), 1666 (vs, ν(C=O)), 2853 (m), 2923 (m), 2956 (m) cm^{-1}.

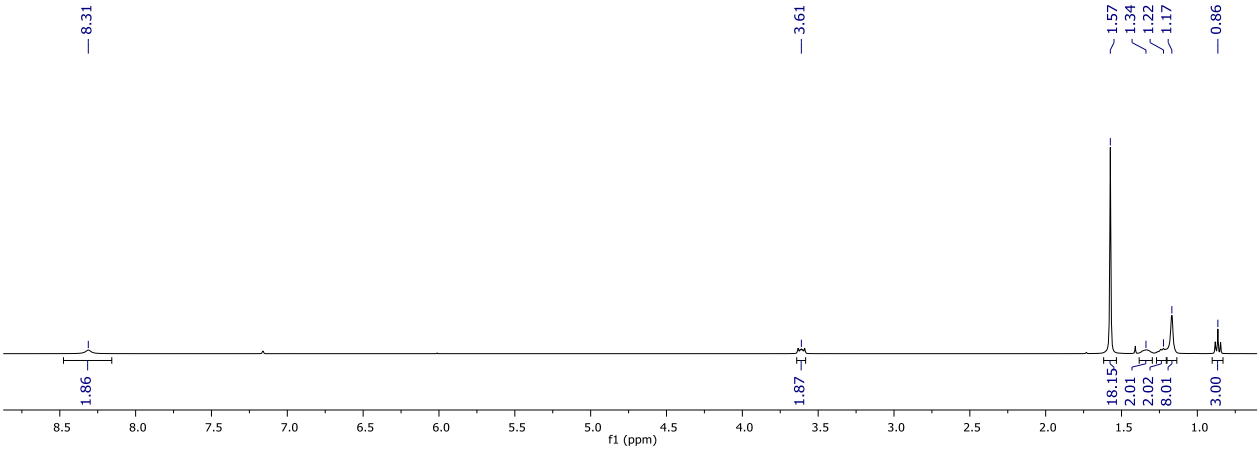


Figure S78: ^{1}H NMR spectrum (in C_6D_6, 300 K, 400.13 MHz) of **6d**.

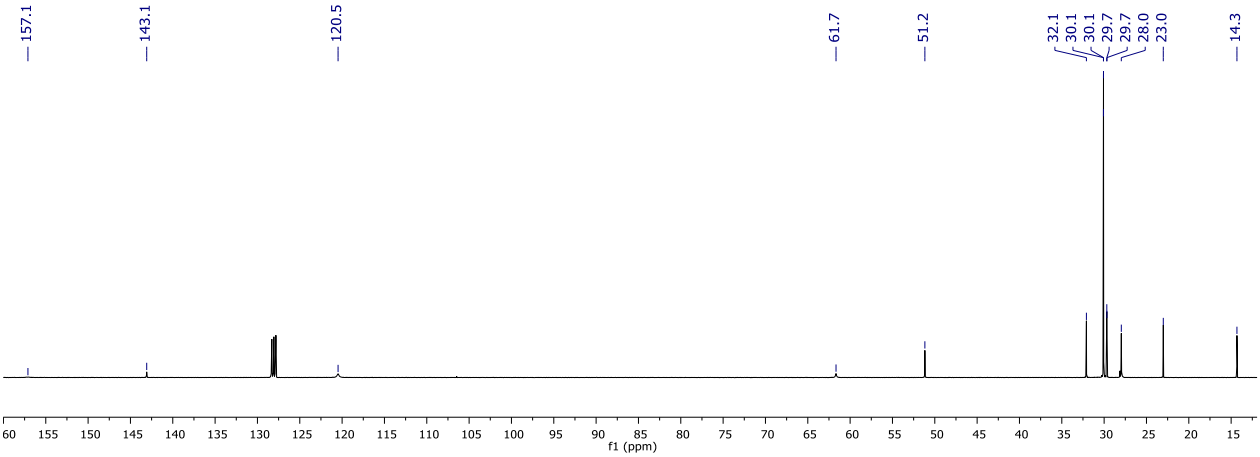
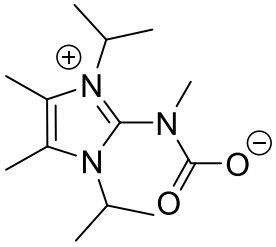


Figure S79: ^{13}C{^{1}H} NMR spectrum (in C_6D_6, 300 K, 100.62 MHz) of **6d**.

Compound 7a: Synthesis according to **GP3** starting from **4a** (0.10 g, 0.48 mmol). Yield 100% (0.12 g, 0.48 mmol) as a white solid.



^{1}H NMR (400.03 MHz, MeCN-d_3): δ = 4.57 (hept, $^{3}J_{HH}$ = 7.1 Hz, 2H, $CH(CH_3)_2$), 2.99 (s, 3H, NCH_3), 2.27 (s, 6H, 2xCH_3), 1.48 (m, 12H, CH_3).

^{13}C{^{1}H} NMR (100.60 MHz, MeCN-d_3): δ = 156.3 (NCO_2), 144.6 (NCN_2), 124.5 (C_q), 50.8 ($NCH(CH_3)_2$), 36.4 (NCH_3), 21.1 ($CHCH_3$), 21.0 ($CHCH_3$), 10.0 (CH_3).

^{15}N NMR (40.55 MHz, MeCN-d_3): δ = 184.9 (NC_3), 70.5 (NCO_2).

HRMS (ESI): m/z calculated for $[C_{12}H_{24}N_3]^+$ $(M\text{-}CO_2+H)^+$ 210.19647, found 210.19685.

IR (neat): $\tilde{\nu}$ = 1092 (m), 1115 (m), 1176 (w), 1225 (m), 1248 (s), 1264 (s), 1366 (w), 1420 (m), 1467 (m), 1545 (w), 1626 (m), 1663 (vs, ν(C=O)), 2881 (m), 2929 (m), 2972 (m) cm^{-1}.

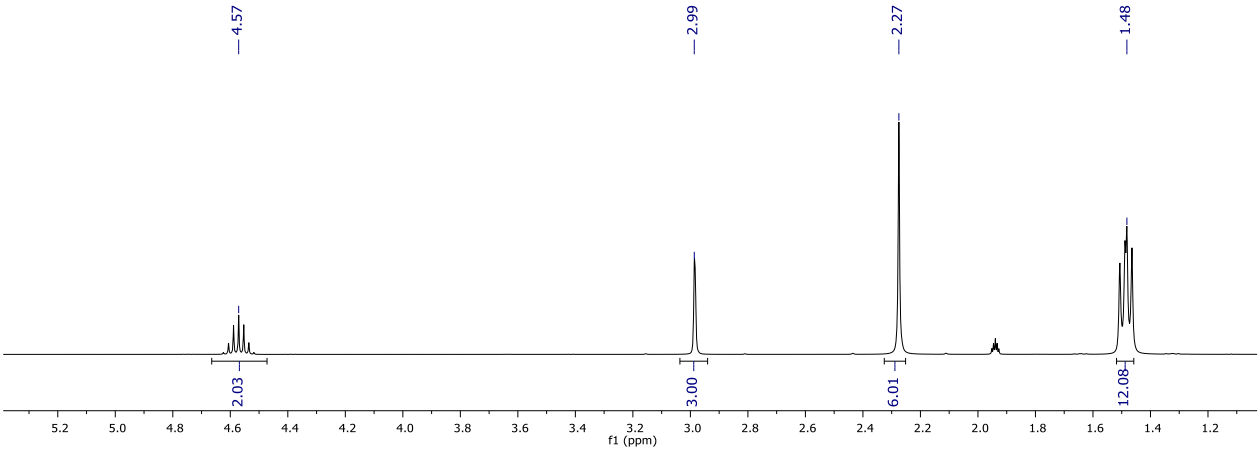


Figure S80: ^{1}H NMR spectrum (in MeCN-d_3, 300 K, 400.03 MHz) of **7a**.

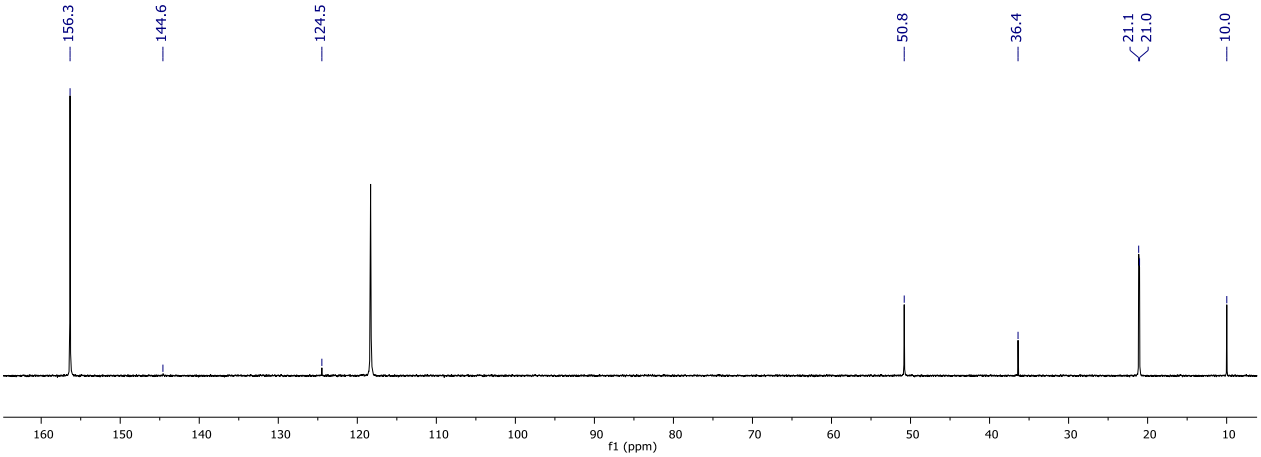


Figure S81: ^{13}C{^{1}H} NMR spectrum (in MeCN-d_3, 300 K, 100.60 MHz) of **7a** prepared using ^{13}C-enriched carbon dioxide gas.

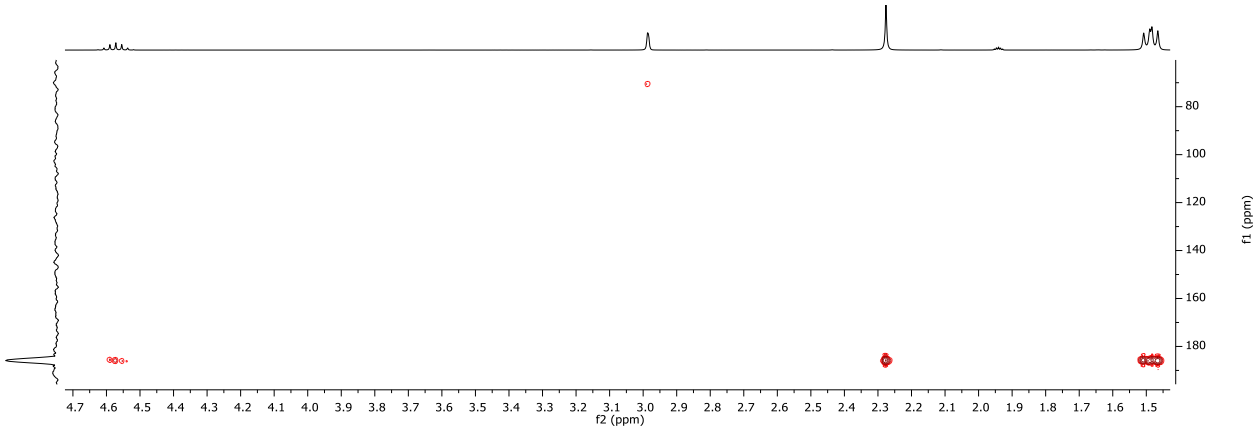
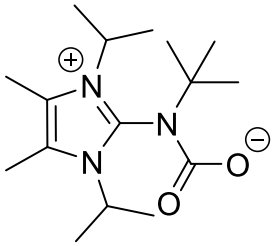


Figure S82: ^{1}H-^{15}N-HMBC NMR spectrum (in MeCN-d_3, 300 K, 400.03, 40.55 MHz) of **7a**.

Compound 7b: Synthesis according to **GP3** starting from **4b** (0.10 g, 0.40 mmol). Yield 100% (0.12 g, 0.40 mmol) as a white solid.



^{1}H NMR (400.03 MHz, $CDCl_3$): δ = 4.79 (hept, $^{3}J_{HH}$ = 7.1 Hz, 2H, $CH(CH_3)_2$), 2.31 (s, 6H, 2xCH_3), 1.55 (d, $^{3}J_{HH}$ = 7.1 Hz, 6H, CH_3), 1.45 (d, $^{3}J_{HH}$ = 7.0 Hz, 6H, CH_3), 1.37 (s, 9H, $C(CH_3)_3$).

^{13}C{^{1}H} NMR (100.62 MHz, $CDCl_3$): δ = 155.7 (NCO_2), 145.0 (NCN_2), 124.5 (C_q), 56.6 ($NC(CH_3)_3$), 50.9 ($NCH(CH_3)_2$), 29.9 (CH_3), 21.0 ($CHCH_3$), 20.8 ($CHCH_3$), 10.4 (CH_3).

HRMS (ESI): m/z calculated for $[C_{15}H_{30}N_3]^+$ $(M\text{-}CO_2+H)^+$ 252.24342, found 252.24313.

IR (neat): $\tilde{\nu}$ = 1040 (w), 1112 (w), 1190 (m), 1219 (m), 1250 (m), 1273 (s), 1391 (m), 1433 (m), 1445 (m), 1512 (m), 1629 (m), 1673 (vs, ν(C=O)), 2952 (m), 2970 (m), 2981 (m) cm^{-1}.

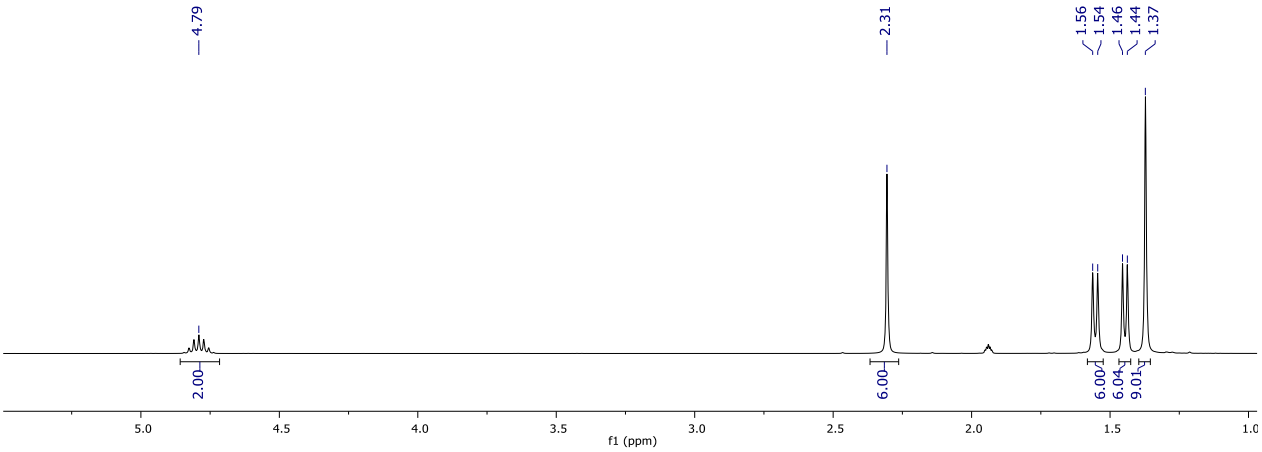


Figure S83: ^{1}H NMR spectrum (in MeCN-d_3, 300 K, 400.03 MHz) of **7b**.

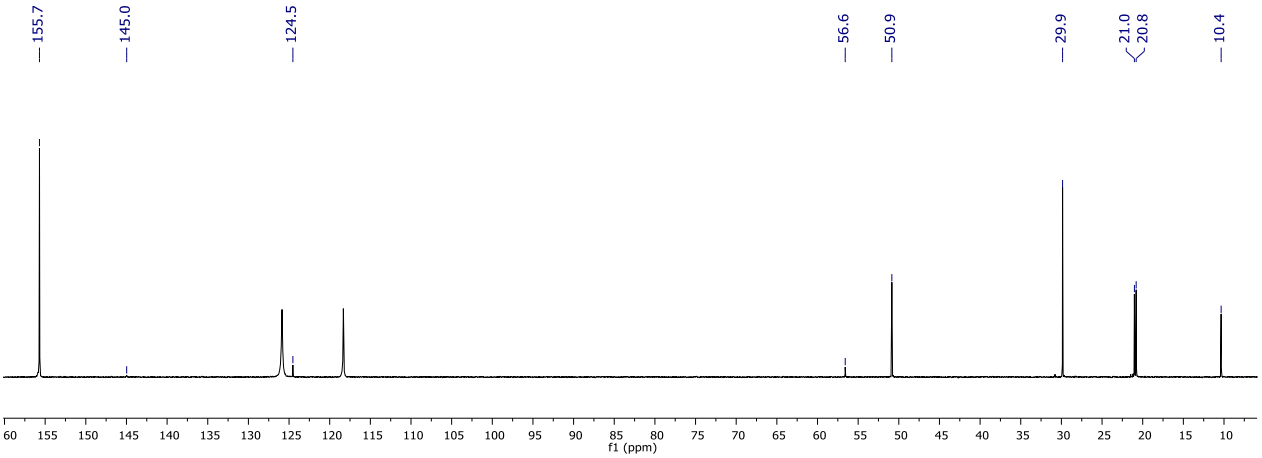
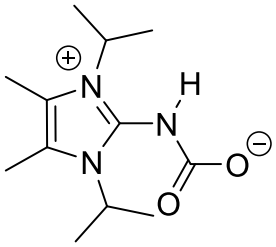


Figure S84: $^{13}C\{^{1}H\}$ NMR spectrum (in MeCN-d_3, 300 K, 100.62 MHz) of **7b** prepared using ^{13}C-enriched carbon dioxide gas.

Compound 7c: Synthesis according to **GP3** starting from **4c** (0.10 g, 0.51 mmol). Yield 100% (0.12 g, 0.51 mmol) as a white solid. For the NMR analysis, **4c** (0.05 g, 0.26 mmol) was dissolved in MeCN-d_3 and the NMR-tube was pressurized with two bar ^{13}C-enriched carbon dioxide.



^{1}H NMR (400.13 MHz, MeCN-d_3): δ = 8.93 (br, 1H, NH), 4.71 (hept, $^{3}J_{HH}$ = 7.0 Hz, 2H, $CH(CH_3)_2$), 2.21 (s, 6H, 2xCH_3), 1.49 (d, $^{3}J_{HH}$ = 7.0 Hz, 12H, 4xCH_3).

$^{13}C\{^{1}H\}$ NMR (100.62 MHz, MeCN-d_3): δ = 143.3 (NCN_2), 138.9 (NCO_2), 122.6 (C_q), 50.0 ($NCH(CH_3)_2$), 21.1 ($CH(CH_3)_2$), 10.0 (CH_3).

$^{13}C\{^{1}H\}$-DEPT135° NMR (100.62 MHz, MeCN-d_3): δ = 50.0 ($NCH(CH_3)_2$), 21.2 ($CH(CH_3)_2$), 10.0 (CH_3).

HRMS (ESI): m/z calculated for $[C_{12}H_{24}N_3]^+$ $(M\text{-}CO_2+H)^+$ 196.18082, found 196.18020.

IR (neat): $\tilde{\nu}$ = 1010 (w), 1097 (w), 1111 (m), 1139 (w), 1171 (w), 1196 (m), 1215 (m), 1277 (vs), 1322 (w), 1370 (m), 1406 (m), 1419 (m), 1453 (m), 1499 (m), 1547 (m), 1599 (s), 1654 (vs, ν(C=O)), 2936 (w), 2978 (m) cm^{-1}.

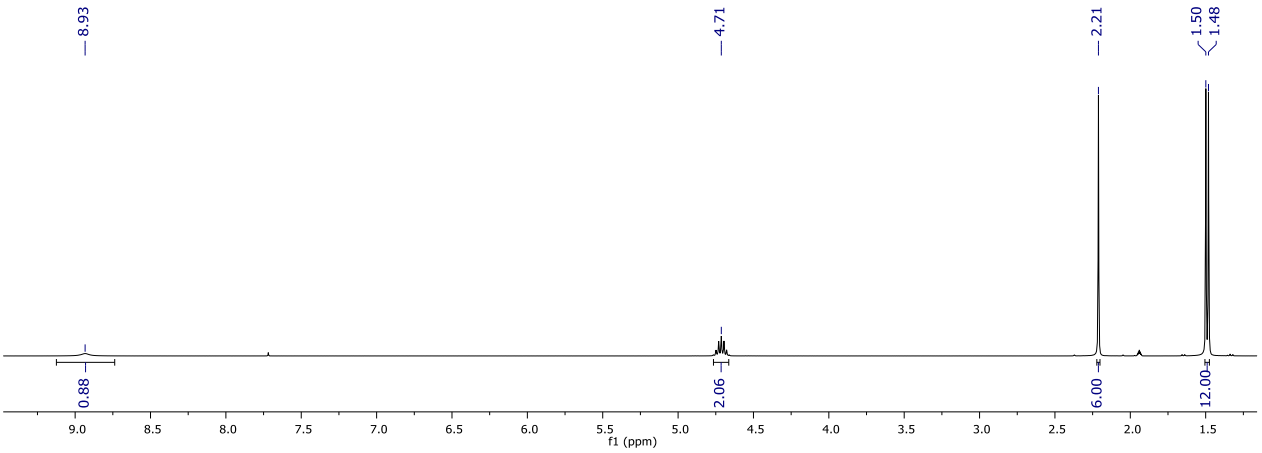


Figure S85: ^{1}H NMR spectrum (in MeCN-d_3, 300 K, 400.13 MHz) of **7c**.

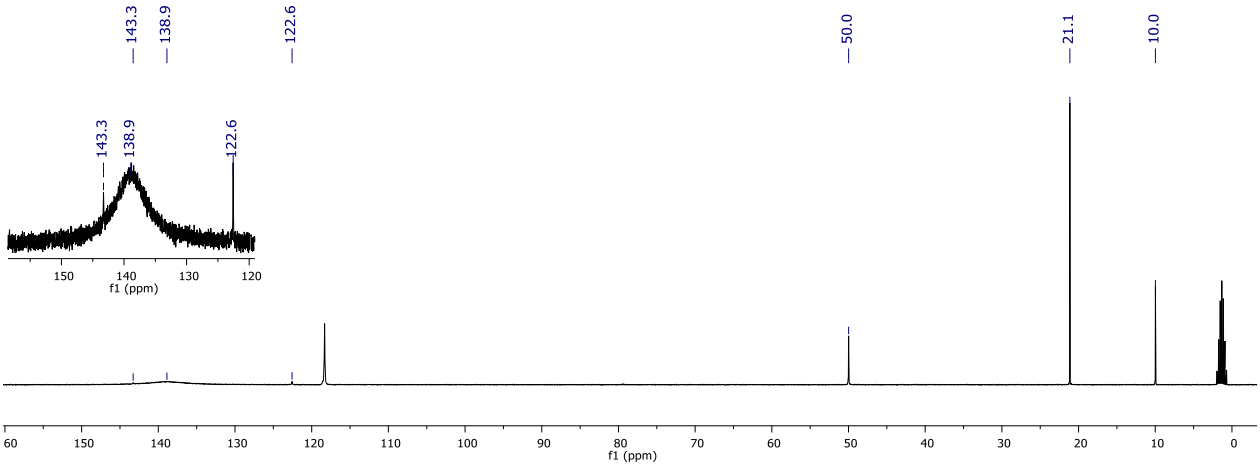


Figure S86: $^{13}C\{^{1}H\}$ NMR spectrum (in MeCN-d_3, 300 K, 100.62 MHz) of **7c** prepared using ^{13}C-enriched carbon dioxide gas.

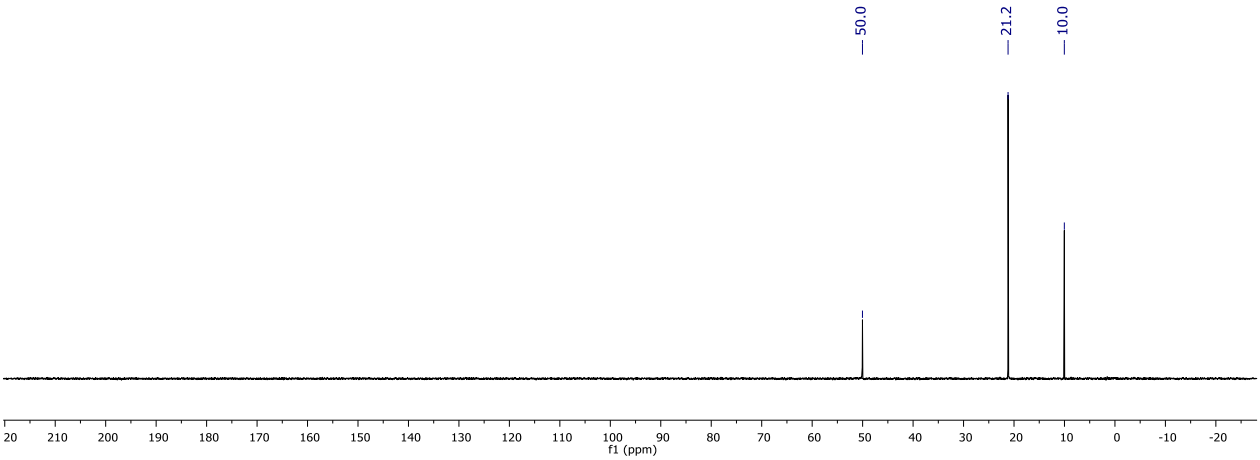
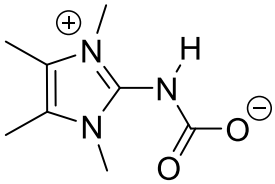


Figure S87: $^{13}C\{^{1}H\}$-DEPT135° NMR spectrum (in MeCN-d_3, 300 K, 100.62 MHz) of **7c**.

Compound 7d: Synthesis according to **GP3** starting from **4d** (0.05 g, 0.36 mmol). Yield 100% (0.07 g, 0.36 mmol) as a white solid.



^{1}H NMR (400.03 MHz, DMSO-d_6/MeCN-d_3): δ = 7.75 (br, 1H, NH), 2.82 (s, 6H, 2xNCH_3), 1.56 (s, 6H, 2xCH_3).

$^{13}C\{^{1}H\}$ NMR (100.60 MHz, DMSO-d_6/MeCN-d_3): δ = 144.5 (NCN_2), 140.6 (NCO_2), 120.9 (C_q), 31.1 (NCH_3), 8.6 (CH_3).

HRMS (ESI): m/z calculated for $[C7H_{14}N_3]^+$ $(M\text{-}CO_2+H)^+$ 140.11822, found 140.11796.

IR (neat): $\tilde{\nu}$ = 1129 (w), 1186 (w), 1251 (s), 1304 (s), 1374 (m), 1435 (m), 1537 (s), 1577 (m), 1615 (s), 1650 (vs, ν(C=O)), 1668 (vs), 2951 (w), 2998 (w), 3227 (m) cm^{-1}.

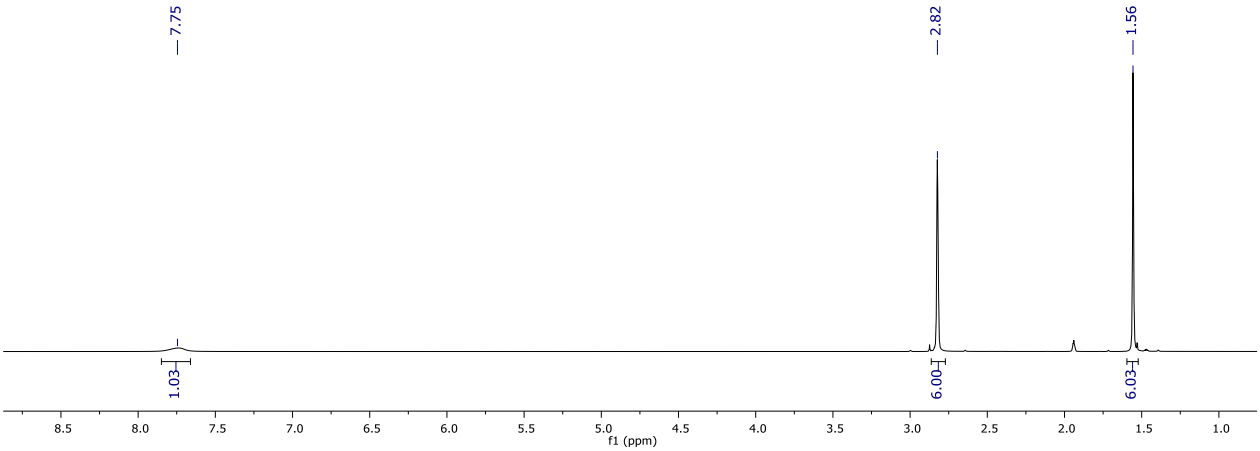


Figure S88: ^{1}H NMR spectrum (in DMSO-d_6/MeCN-d_3, 300 K, 400.03 MHz) of **7d**.

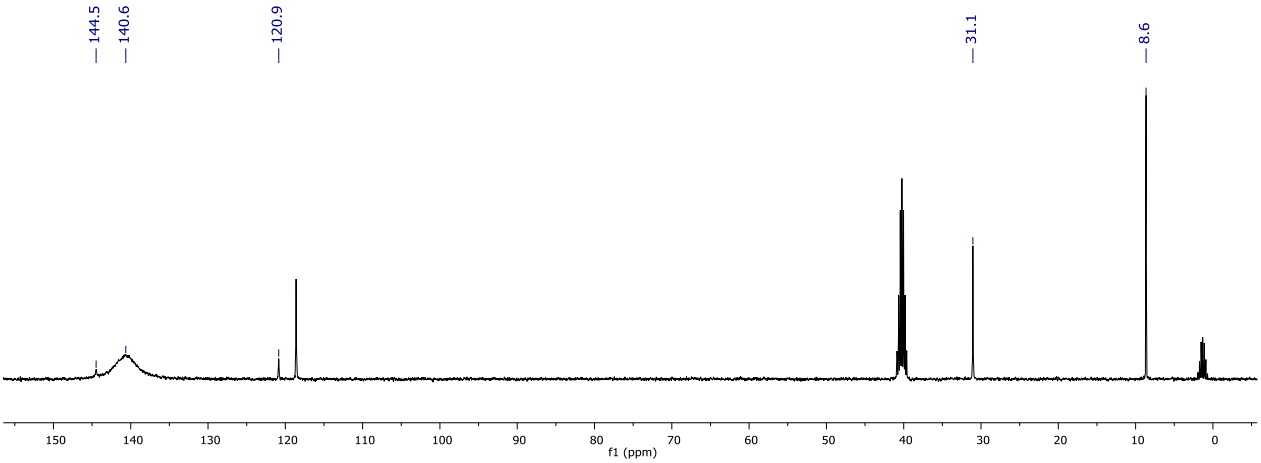
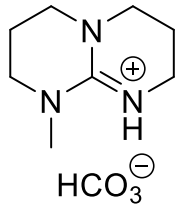


Figure S89: ^{13}C{^{1}H} NMR spectrum (in DMSO-d_6/MeCN-d_3, 300 K, 100.60 MHz) of **7d** prepared using ^{13}C-enriched carbon dioxide gas.

Synthesis of bicarbonates [MTBDH][HCO_3] and [DBNH][HCO_3]

[MTBDH][HCO_3]: MTBD (0.02 g, 0.10 mmol) was dissolved in hydrous MeCN and the solution was pressurized with two bar ^{13}C-labeled carbon dioxide pressure. A colorless precipitate formed which was separated from the solution. Yield 100% (0.02 g, 0.10 mmol) as a colorless solid. Owing to the low solubility of [MTBDH][HCO_3] in MeCN or DMSO, the NMR analysis was performed in D_2O.



^{1}H NMR (400.13 MHz, D_2O): δ = 3.20 (m, 8H, CH_2), 2.82 (s, 3H, CH_3), 1.89 (p, $^3J_{HH}$ = 6.0 Hz, 2H, CH_2), 1.84 (p, $^3J_{HH}$ = 5.9 Hz, 2H, CH_2).

^{13}C{^{1}H} NMR (100.62 MHz, D_2O): δ = 160.7 (HCO_3^-), 151.9 (CN_3), 48.6 (CH_2), 48.1 (CH_2), 47.6 (CH_2), 39.4 (CH_3), 37.3 (CH_2), 21.3 (CH_2), 21.1 (CH_2).

HRMS (ESI): m/z calculated for $[C_8H_{16}N_3]^+$ $(M)^+$ 154.13387, found 154.13354.

IR (neat): $\tilde{\nu}$ = 989 (s), 1017 (w), 1045 (m), 1093 (m), 1105 (w), 1130 (m), 1182 (s), 1218 (s), 1257 (s), 1290 (s), 1309 (vs), 1320 (vs), 1353 (vs), 1421 (w), 1445 (m), 1477 (m), 1510 (m), 1592 (vs, $\nu(HCO_3^-)$, 1636 (m), 2875 (w) cm^{-1}.

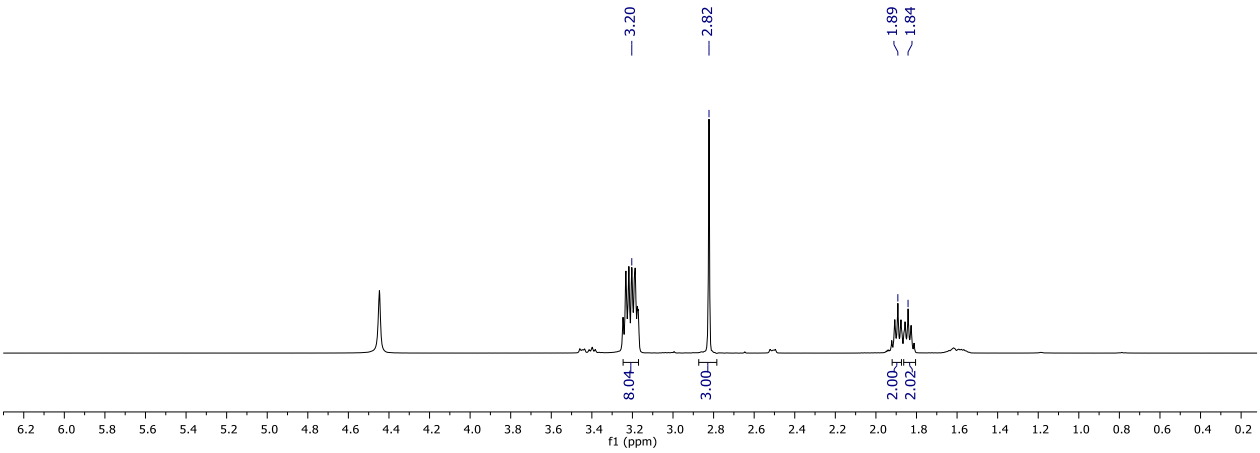


Figure S90: ^{1}H NMR spectrum (in D_2O, 300 K, 400.13 MHz) of [MTBDH][HCO_3].

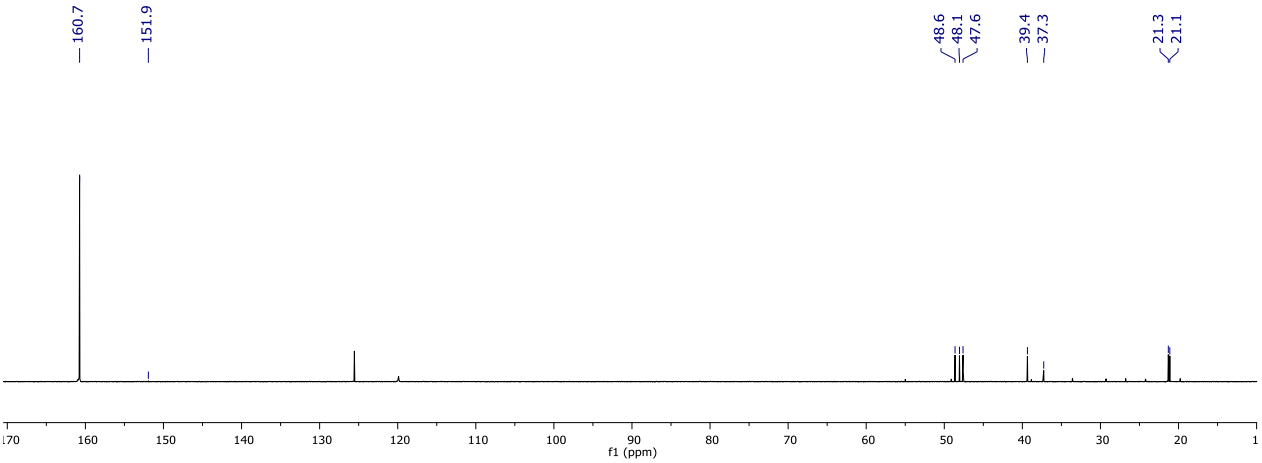
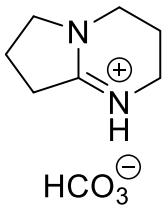


Figure S91: $^{13}C\{^{1}H\}$ NMR spectrum (in D_2O, 300 K, 100.62 MHz) of [MTBDH][HCO_3] prepared using ^{13}C-enriched carbon dioxide gas.

[DBNH][HCO_3]: DBN (0.01 g, 0.10 mmol) was dissolved in hydrous MeCN-d_3 and the NMR-tube was pressurized with two bar ^{13}C-labeled carbon dioxide pressure. According to the NMR analysis [DBNH][HCO_3] formed in quantitative yield.



^{1}H NMR (400.13 MHz, MeCN-d_3): δ = 5.74 (br, 2H, NH/HCO_3^-), 3.55 (t, $^{3}J_{HH}$ = 7.2 Hz, 2H, CH_2), 3.33 (s, 4H, CH_2), 2.85 (t, $^{3}J_{HH}$ = 8.0 Hz, 2H, CH_2), 2.06 (m, 2H, CH_2), 1.94 (p, $^{3}J_{HH}$ = 6.0 Hz, 2H, CH_2).

$^{13}C\{^{1}H\}$ NMR (100.62 MHz, MeCN-d_3): δ = 165.3 (CCN_2), 161.9 (HCO_3^-), 53.9 (CH_2CN), 43.2 (CH_2CN), 39.0 (CH_2CN), 30.8 (CH_2C_qC), 19.6 (CH_2), 19.6 (CH_2).

HRMS (ESI): m/z calculated for $[C_7H_{13}N_2]^+$ $(M)^+$ 125.10733, found 125.10693.

IR (neat): $\tilde{\nu}$ = 966 (m), 1006 (m), 1063 (m), 1115 (w), 1133 (m), 1175 (m), 1194 (m), 1206 (m), 1229 (w), 1308 (vs), 1352 (vs), 1385 (s), 1425 (w), 1444 (w), 1476 (w), 1592 (vs, $\nu(HCO_3^-)$, 1632 (s), 1673 (m), 2609 (w), 2680 (w), 2889 (w) cm^{-1}.

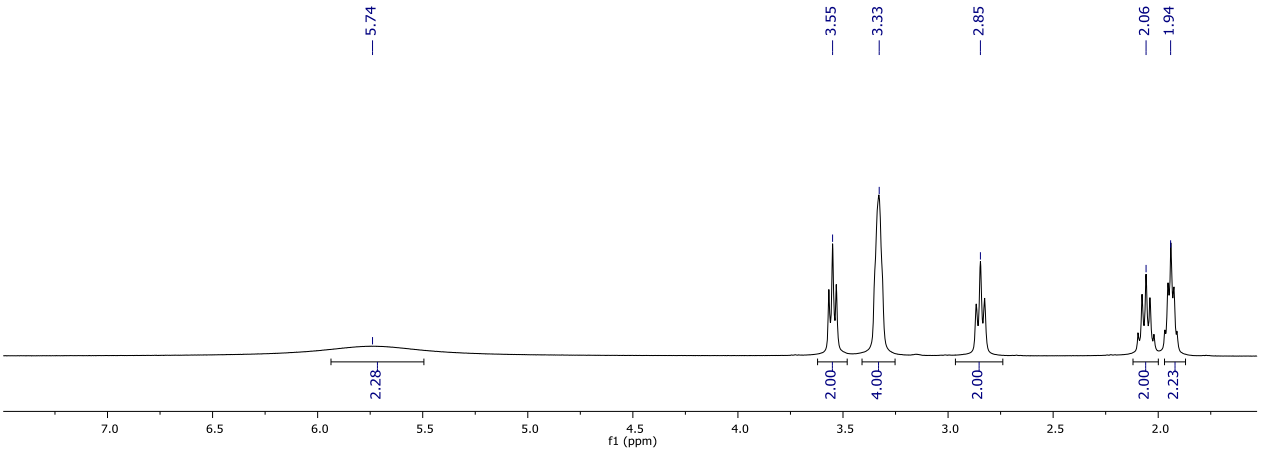


Figure S92: ^{1}H NMR spectrum (in MeCN-d_3, 300 K, 400.13 MHz) of [DBNH][HCO_3].

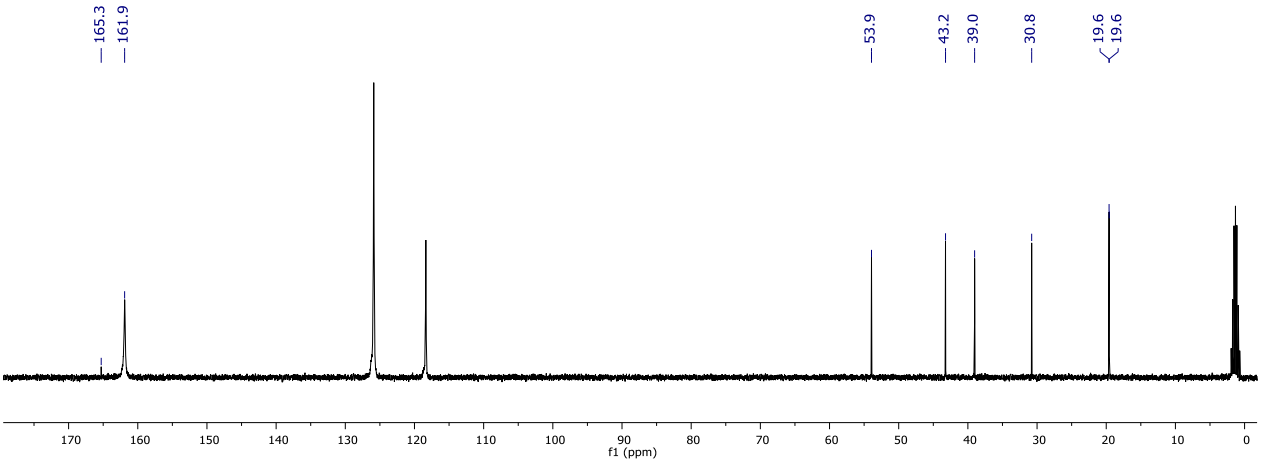


Figure S93: $^{13}C\{^{1}H\}$ NMR spectrum (in MeCN-d_3, 300 K, 100.62 MHz) of [DBNH][HCO_3] prepared using ^{13}C-enriched carbon dioxide gas.

Stability of NHI–CO_2 adduct (I^tBu)N^tBuCO_2 (**6b**)

The stability of NHI–CO_2 adduct (I^tBu)N^tBuCO_2 (**6b**) was examined by ^1H and ^{13}C NMR spectroscopy. **3b** (0.03 g, 0.12 mmol) was dissolved in MeCN-d_3 and the NMR tube was pressurized with 2 bar $^{13}CO_2$. The reaction mixture was immediately analyzed by NMR spectroscopy revealing the formation of adduct **6b**. After storing the NMR tube for 4 h at room temperaure, the NMR analysis showed 29% conversion of **6b** into *tert*-butyl isocyanate and 1,3-di-*tert*-butyl-2-imidazolinone. Full conversion was observed after heating a solution of **6b** in MeCN to 50 °C for 3 h.

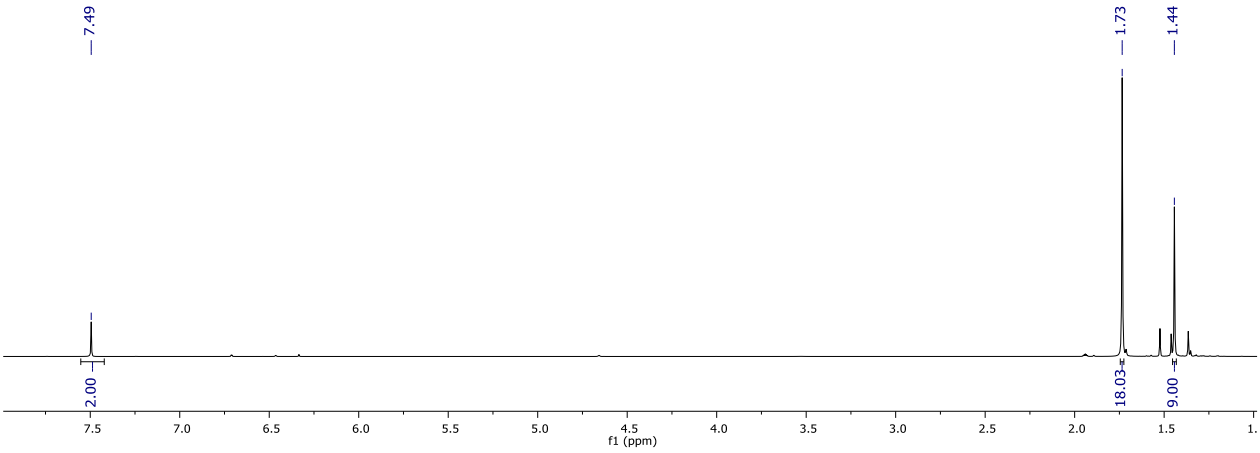


Figure S94: ^1H NMR spectrum (in MeCN-d_3, 300 K, 400.03 MHz) of **6b**.

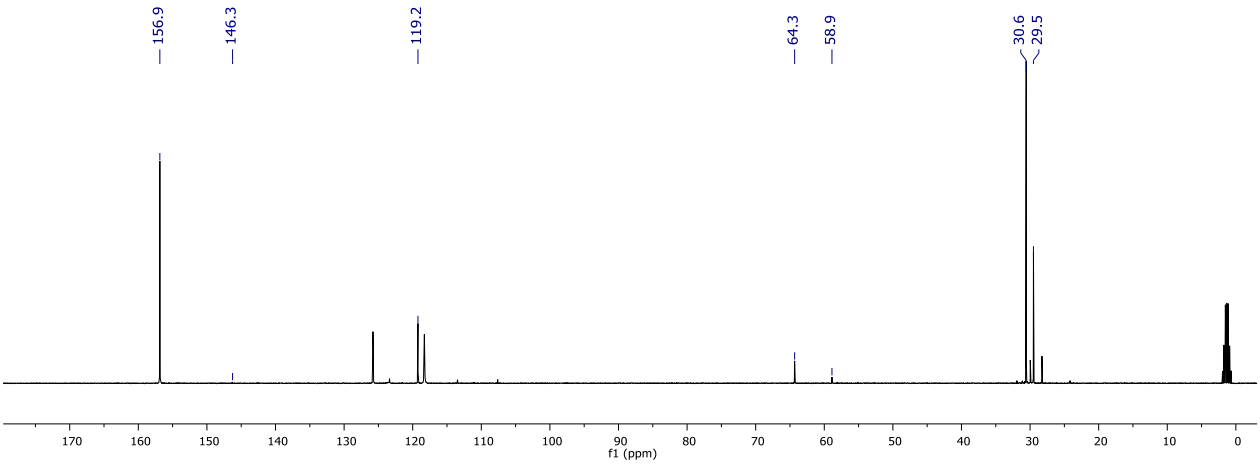


Figure S95: $^{13}C\{^1H\}$ NMR spectrum (in MeCN-d_3, 300 K, 100.60 MHz) of **6b** prepared using ^{13}C-enriched carbon dioxide gas (The resonance at 125.8 ppm corresponds to $^{13}CO_2$).

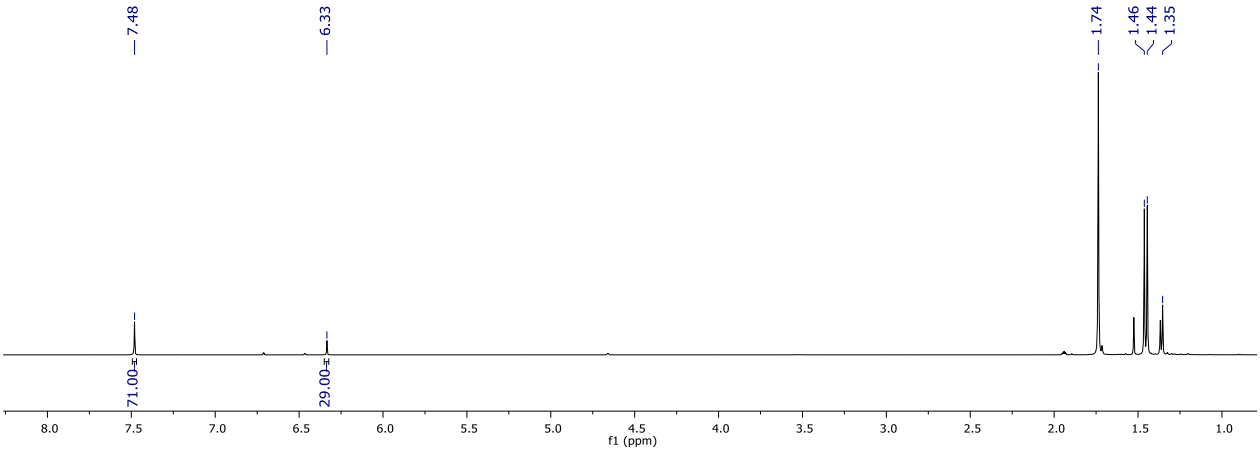


Figure S96: ^{1}H NMR spectrum (in MeCN-d_3, 300 K, 400.03 MHz) after storing a solution of **6b** for 4 h at room temperature (**6b**: 7.48, 1.74, 1.44 ppm; 1,3-di-*tert*-butyl-2-imidazolinone: 6.33, 1.46 ppm; *tert*-butyl isocyanate: 1.35 ppm).

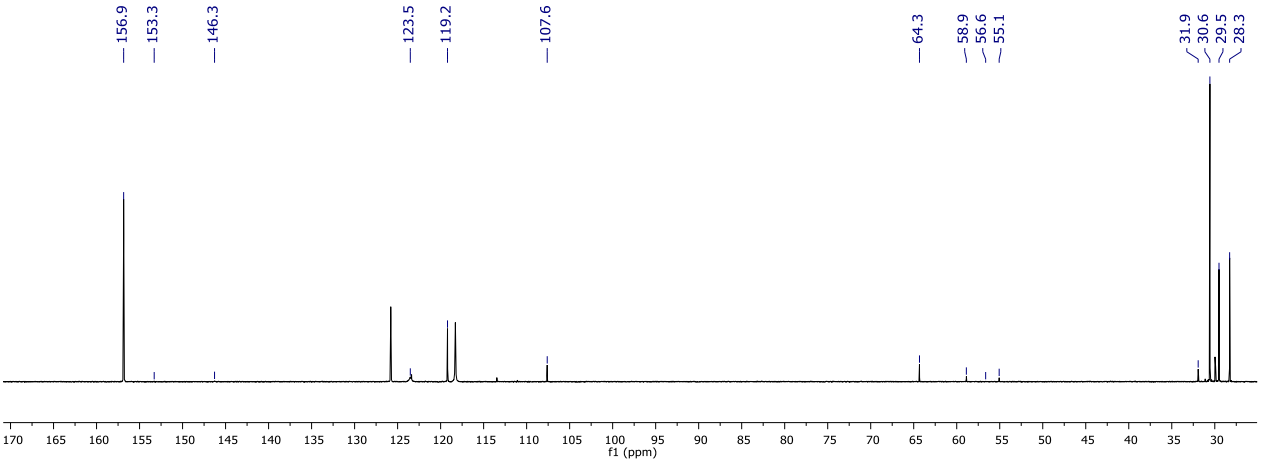


Figure S97: ^{13}C{^{1}H} NMR spectrum (in MeCN-d_3, 300 K, 100.60 MHz) after storing a solution of **6b** for 4 h at room temperature (**6b**: 156.9, 146.3, 119.2, 64.3, 58.9, 30.6, 29.5 ppm; 1,3-di-*tert*-butyl-2-imidazolinone: 153.3, 107.6, 55.1, 28.3 ppm; *tert*-butyl isocyanate: 123.5, 56.6, 31.9 [d, $^{3}J_{CC}$ = 2.0 Hz] ppm).

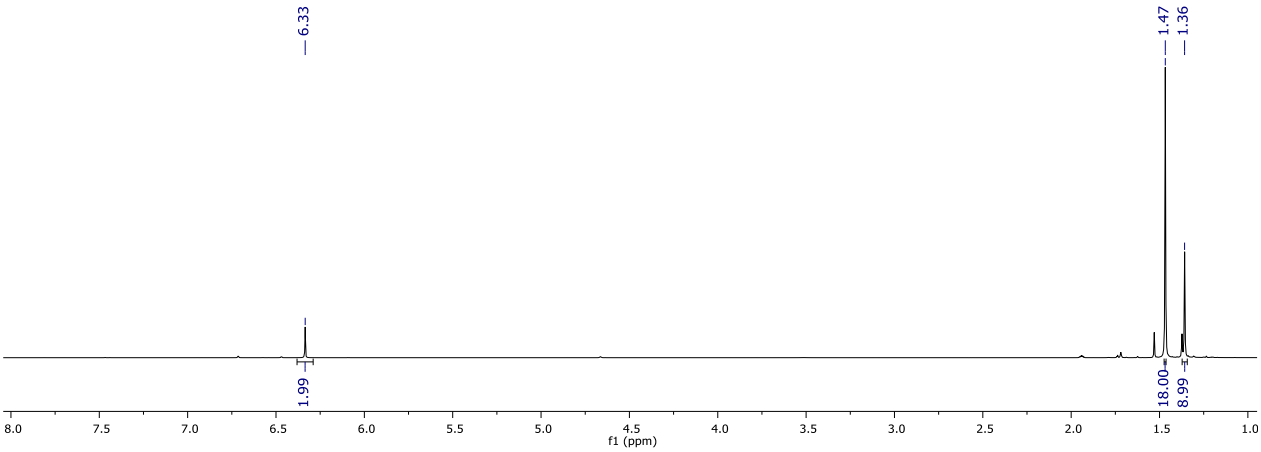


Figure S98: ^{1}H NMR spectrum (in MeCN-d_3, 300 K, 400.03 MHz) after heating a solution of **6b** for 3 h at 50 °C (**6b**: -; 1,3-di-*tert*-butyl-2-imidazolinone: 6.33, 1.47 ppm; *tert*-butyl isocyanate: 1.36 ppm).

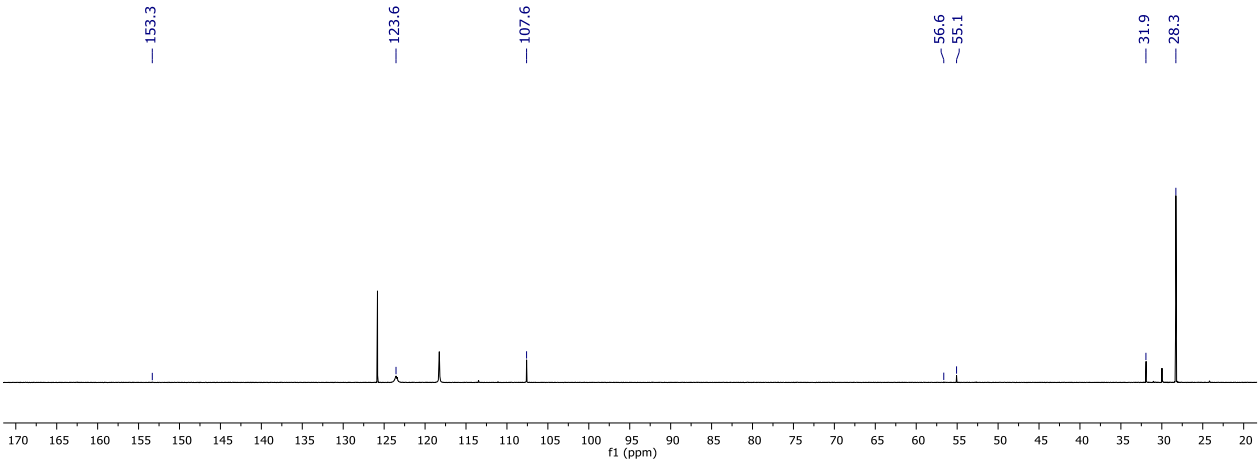


Figure S99: $^{13}C\{^{1}H\}$ NMR spectrum (in MeCN-d_3, 300 K, 100.60 MHz) after heating a solution of **6b** for 3 h at 50 °C (**6b**: -; 1,3-di-*tert*-butyl-2-imidazolinone: 153.3, 107.6, 55.1, 28.3 ppm; *tert*-butyl isocyanate: 123.5, 56.6 [d, $^{2}J_{CC}$ = 2.8 Hz], 31.9 [d, $^{3}J_{CC}$ = 2.0 Hz] ppm).

Experiments towards the hydrolysis of nitrogen base–CO_2 adducts

The stability of the nitrogen base–CO_2 adducts towards hydrolysis was examined by the following procedure:

Water was added to a solution of the respective N-heterocyclic imine– or amidine–CO_2 adduct (0.1 mmol) in acetonitrile in portions of 5 µL (2.7 eq.) using a Hamilton Syringe. The conversion of the CO_2 adduct to give the bicarbonate salt was determined by ^{1}H NMR analysis of the reaction mixture using the C–H protons of the imidazoline ring (**6a-d**) or the C–H protons of the isopropyl group at the imidazoline-N atoms (**7**).

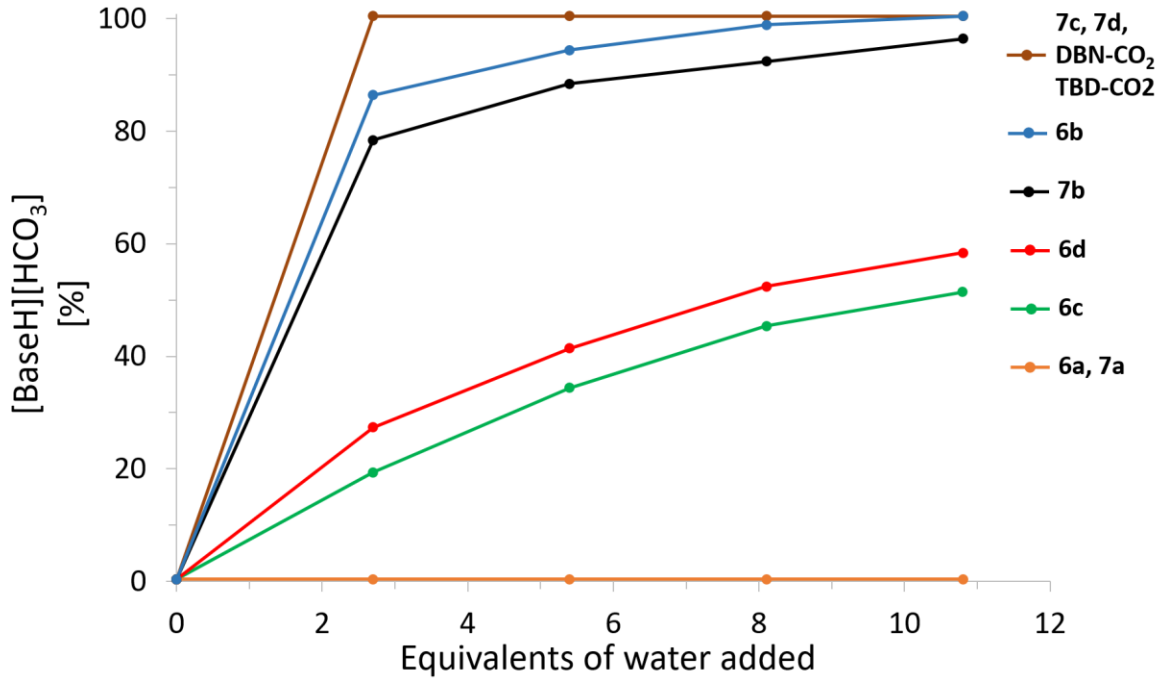


***Figure S100*:** Conversion of selected nitrogen base–CO_2 adducts into the corresponding bicarbonate salts upon addition of water to a MeCN-d_3 solution of the CO_2 adduct.

Table S2: Conversion of selected nitrogen base–CO_2 adducts into the corresponding bicarbonate salts upon addition of water to a MeCN solution of the CO_2 adduct. Full conversion to the bicarbonates [baseH][HCO_3] was observed upon addition of 2.7 eq. of water for CO_2 adducts **7c**, **7d**, TBD-CO_2 and DBN-CO_2 (**1**).

Water [eq.]	[**6a**H][HCO_3] [%]	[**6b**H][HCO_3] [%]	[**6c**H][HCO_3] [%]	[**6d**H][HCO_3] [%]	[**7a**H][HCO_3] [%]	[**7b**H][HCO_3] [%]
2.7	0	86	19	27	0	78
5.4	0	94	34	41	0	88
8.1	0	99	45	52	0	92
10.8	0	100	51	58	0	96

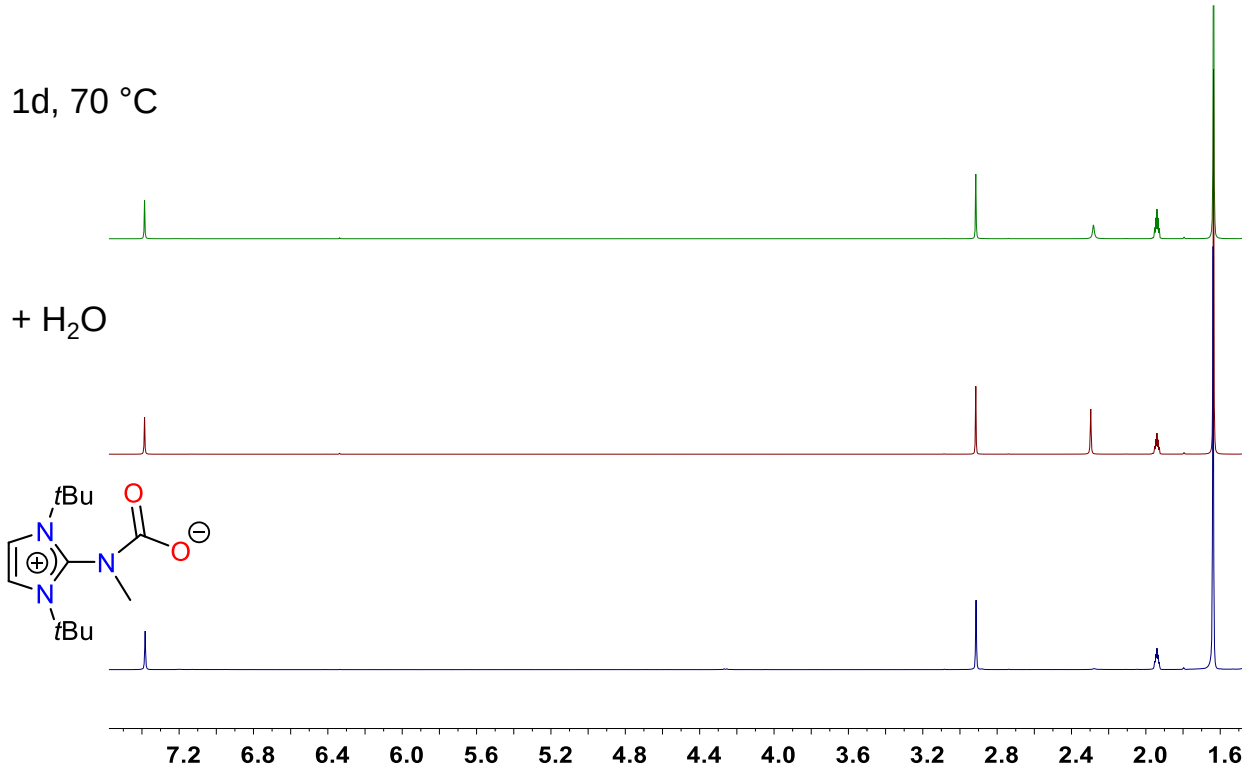


***Figure S101*:** ^{1}H NMR spectra (in MeCN-d_3, 300 K, 400.03 MHz) of **6a** (bottom), after the addition of H_2O (middle) and after heating the sample for 24 h at 70 °C (top).

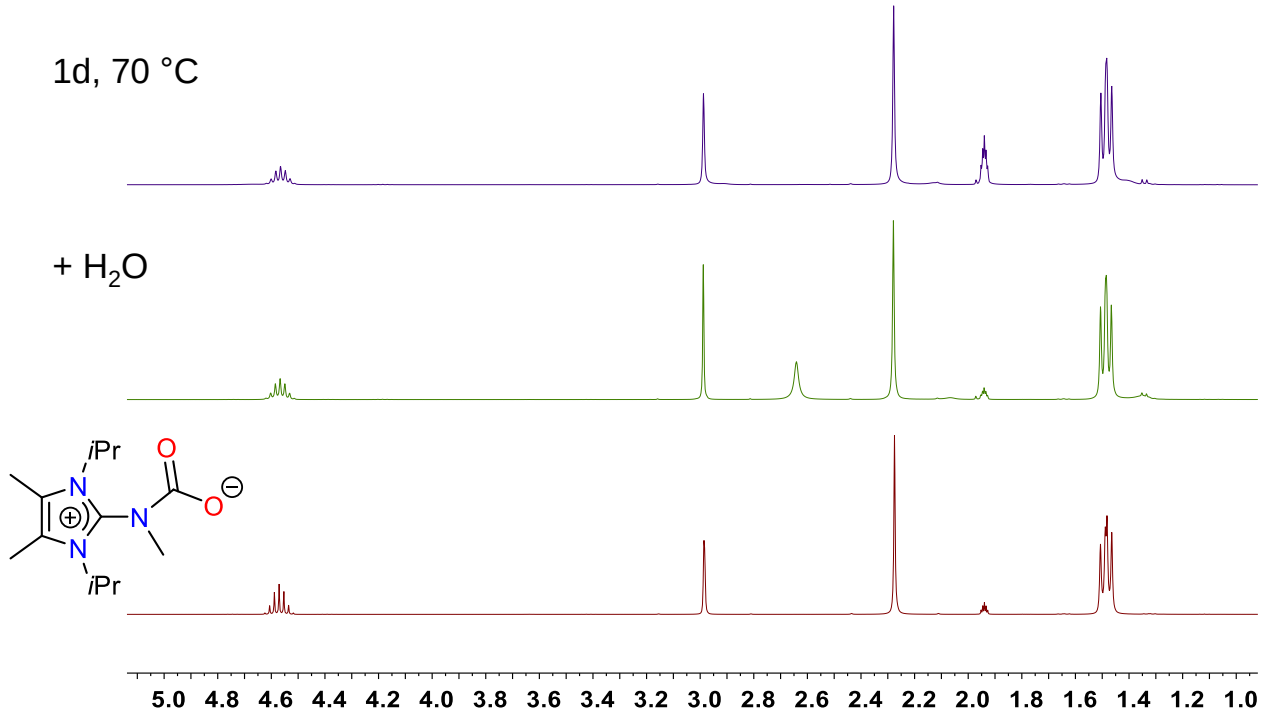


***Figure S102*:** ^{1}H NMR spectra (in MeCN-d_3, 300 K, 400.03 MHz) of **7a** (bottom), after the addition of H_2O (middle) and after heating the sample for 24 h at 70 °C (top).

X-ray Diffraction Studies

General: Single-crystal X-ray diffraction data were collected on a Bruker AXS detector using Mo-K_α radiation (λ = 0.71073 Å). Crystals were selected under oil, mounted on nylon loops and then immediately placed in a cold stream of N_2 on a diffractometer. Using Olex2,[23] the structures were solved with the Superflip[24] structure solution program using Charge Flipping and refined with the ShelXL[25] refinement package using Least Squares minimization.

Ellipsoids are drawn at 50% probability. If present, solvent molecules and disordered parts are shown for a complete structural depiction.

Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-1866029 (**1**), CCDC-1866030 ([**1**H][HCO_3]), CCDC-1866031 (**6a**), CCDC-1866032 (**2c**), CCDC-1866033 (**7c**), CCDC-1866034 ([MTBDH][HCO_3]), CCDC-1866035 (**7d**), CCDC-1866036 (**4e**), CCDC-1866037 (**7b**), CCDC-1866038 (**6c**), CCDC-1866039 (**7a**), CCDC-1880247 ([**3b**H][BF_4]) and CCDC-1880248 (**6b**). These data can be obtained free of charge via www.ccdc.cam.uk/data_request/cif (or from the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

Single-crystal X-ray structure analysis of 1:

Single crystals were obtained by pressuring an Et_2O solution of DBN with two bar CO_2 pressure. A Single-crystal X-ray structure analysis revealed that **1** crystallizes in the orthorhombic space group *Pca*2_1. The asymmetric unit contains one molecule of **1**.

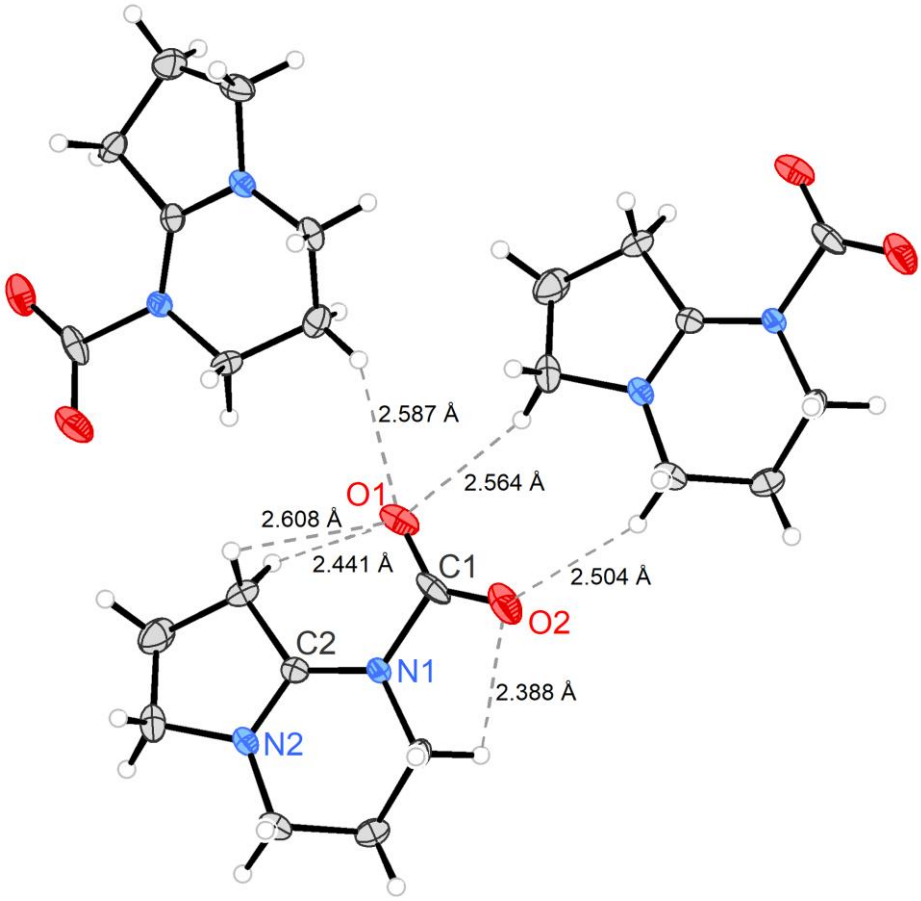


Figure S103: Molecular view of **1** in the solid state illustrating short O···H contacts.

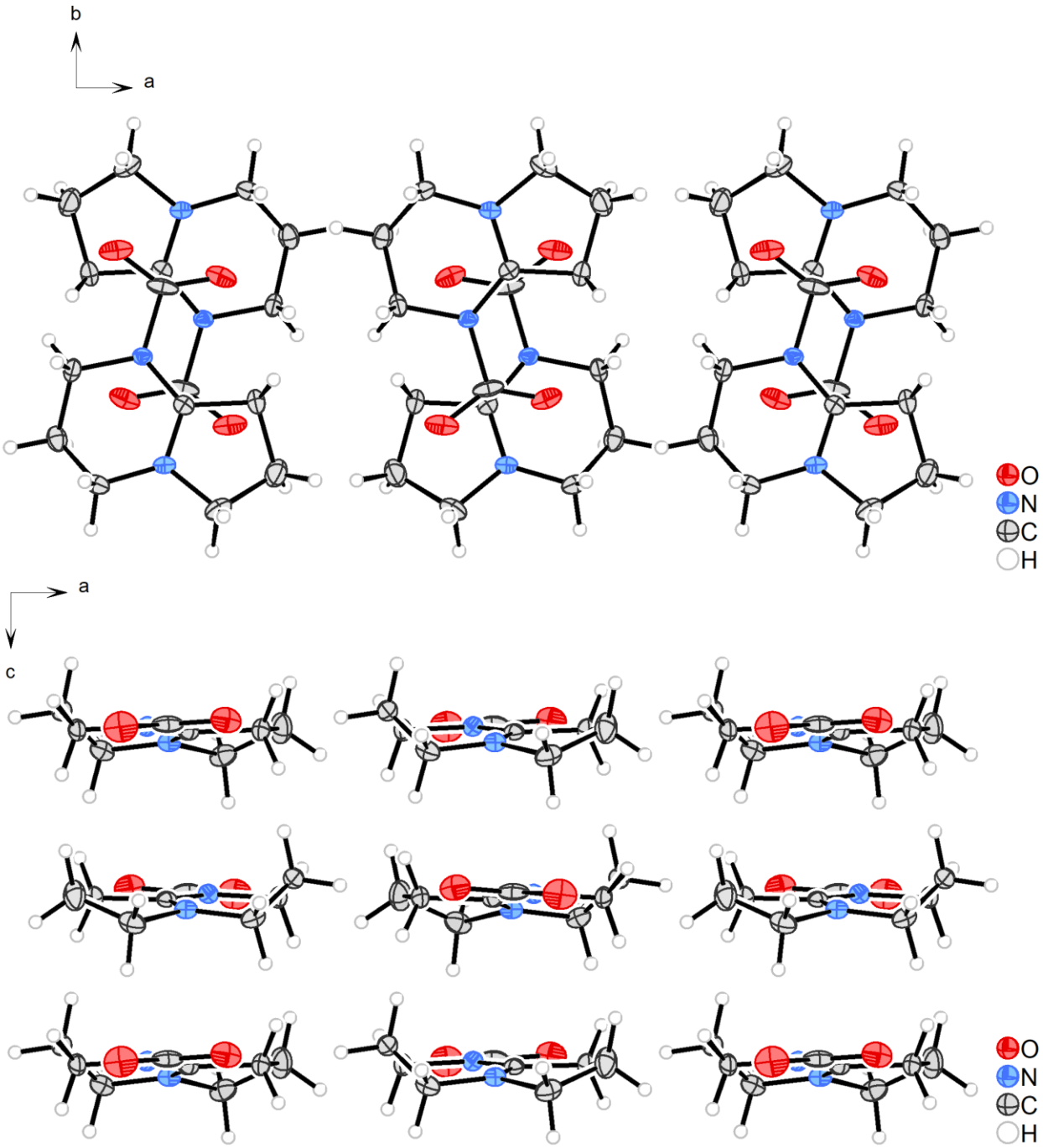


Figure S104: Molecular view of **1** in the solid state along the crystallographic *c* axis (top) and *b* axis (bottom), illustrating the packing of **1**.

Table S3. Crystal data and structure refinement for **1**.

CCDC Number	1866029
Empirical formula	$C_8H_{12}N_2O_2$
Formula weight	168.20
Temperature/K	99.97
Crystal system	orthorhombic

Space group	$Pca2_1$
a/Å	13.4813(4)
b/Å	8.2397(3)
c/Å	6.9346(2)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	770.31(4)
Z	4
ρ_{calc}g/cm^3	1.450
μ/mm^{-1}	0.106
F(000)	360.0
Crystal size/mm^3	0.6 × 0.163 × 0.137
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.944 to 56.808
Index ranges	$-17 \leq h \leq 17$, $-10 \leq k \leq 10$, $-9 \leq l \leq 9$
Reflections collected	10967
Independent reflections	1901 [R_{int} = 0.0262, R_{sigma} = 0.0183]
Data/restraints/parameters	1901/1/109
Goodness-of-fit on F^2	1.120
Final R indexes [I>=2σ (I)]	R_1 = 0.0448, wR_2 = 0.1153
Final R indexes [all data]	R_1 = 0.0459, wR_2 = 0.1162
Largest diff. peak/hole / e Å^{-3}	0.55/-0.20
Flack parameter	0.2(4)

Single-crystal X-ray structure analysis of [DBNH][HCO_3]:

Single crystals were obtained by pressuring a wet C_6D_6 solution of **1** with two bar CO_2 pressure. A Single-crystal X-ray structure analysis revealed that [DBNH][HCO_3] crystallizes in the monoclinic space group $P2_1/n$. The asymmetric unit contains one molecule of [DBNH][HCO_3].

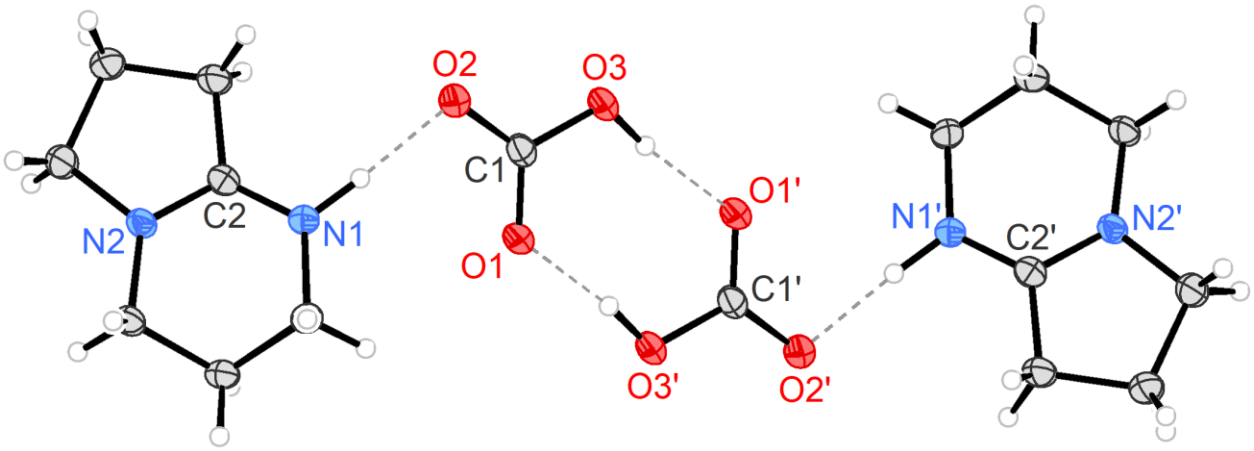


Figure S105: Molecular view of [DBNH][HCO_3] in the solid state.

Table S4. Crystal data and structure refinement for [DBNH][HCO_3].

CCDC Number	1866030
Empirical formula	$C_8H_{14}N_2O_3$
Formula weight	186.21
Temperature/K	100
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	7.7428(6)
b/Å	11.1556(9)
c/Å	10.4925(8)
α/°	90
β/°	98.8440(10)
γ/°	90
Volume/Å^3	895.52(12)
Z	4
ρ_{calc}g/cm^3	1.381
μ/mm^{-1}	0.106
F(000)	400.0
Crystal size/mm^3	0.231 × 0.127 × 0.075
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.364 to 52.768
Index ranges	$-9 \le h \le 8$, $-13 \le k \le 13$, $-13 \le l \le 13$
Reflections collected	4119
Independent reflections	1726 [R_{int} = 0.0145, R_{sigma} = 0.0178]
Data/restraints/parameters	1726/0/126
Goodness-of-fit on F^2	1.043
Final R indexes [I>=2σ (I)]	R_1 = 0.0385, wR_2 = 0.0956
Final R indexes [all data]	R_1 = 0.0412, wR_2 = 0.0977
Largest diff. peak/hole / e Å^{-3}	0.29/-0.19

Single-crystal X-ray structure analysis of [MTBDH][HCO_3]:

Single crystals were obtained by pressuring a wet C_6D_6 solution of MTBD with two bar CO_2 pressure. A Single-crystal X-ray structure analysis revealed that [MTBDH][HCO_3] crystallizes in the monoclinic space group $P2_1/n$. The asymmetric unit contains one molecule of [MTBDH][HCO_3].

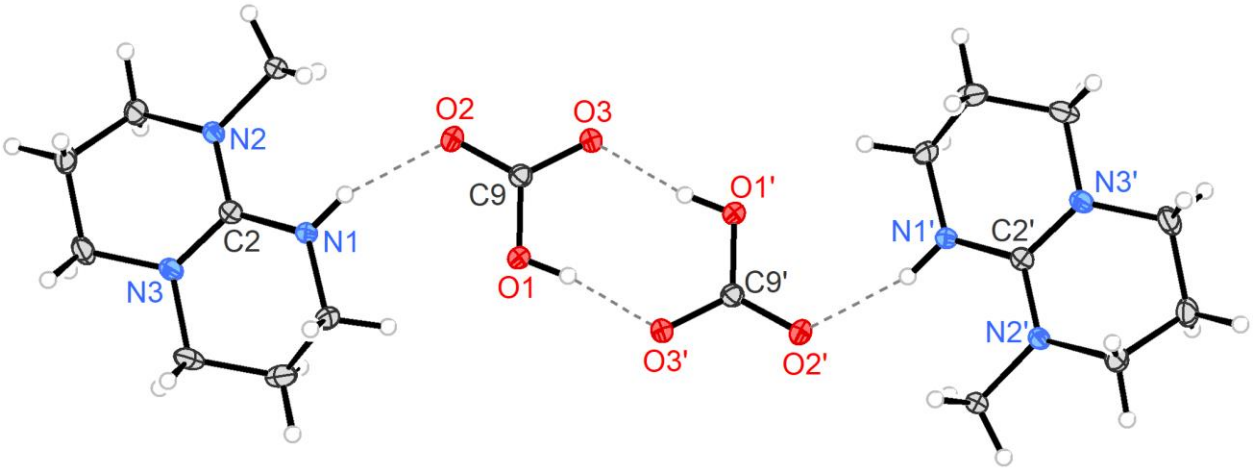


Figure S106: Molecular view of [MTBDH][HCO_3] in the solid state.

Table S5. Crystal data and structure refinement for [MTBDH][HCO_3].

CCDC Number	1866034
Empirical formula	$C_9H_{17}N_3O_3$
Formula weight	215.25
Temperature/K	100
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	8.14690(10)
b/Å	10.06590(10)
c/Å	12.9174(2)
α/°	90
β/°	104.7990(10)
γ/°	90
Volume/Å^3	1024.16(2)
Z	4
ρ_{calc}g/cm^3	1.396
μ/mm^{-1}	0.106
F(000)	464.0
Crystal size/mm^3	0.058 × 0.081 × 0.135
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.198 to 56.598
Index ranges	$-10 \le h \le 10$, $-13 \le k \le 13$, $-17 \le l \le 16$
Reflections collected	14847
Independent reflections	2537 [R_{int} = 0.0279, R_{sigma} = 0.0192]
Data/restraints/parameters	2537/0/138
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0382, wR_2 = 0.0959
Final R indexes [all data]	R_1 = 0.0448, wR_2 = 0.0999
Largest diff. peak/hole / e Å^{-3}	0.30/-0.22

Single-crystal X-ray structure analysis of 2c:

Single crystals were obtained by slow cooling of a saturated *n*-hexane solution of **2c** under CO_2 atmosphere. A Single-crystal X-ray structure analysis revealed that **2c** crystallizes in the orthorhombic space group $P2_12_12_1$. The asymmetric unit contains two molecules of **2c**.

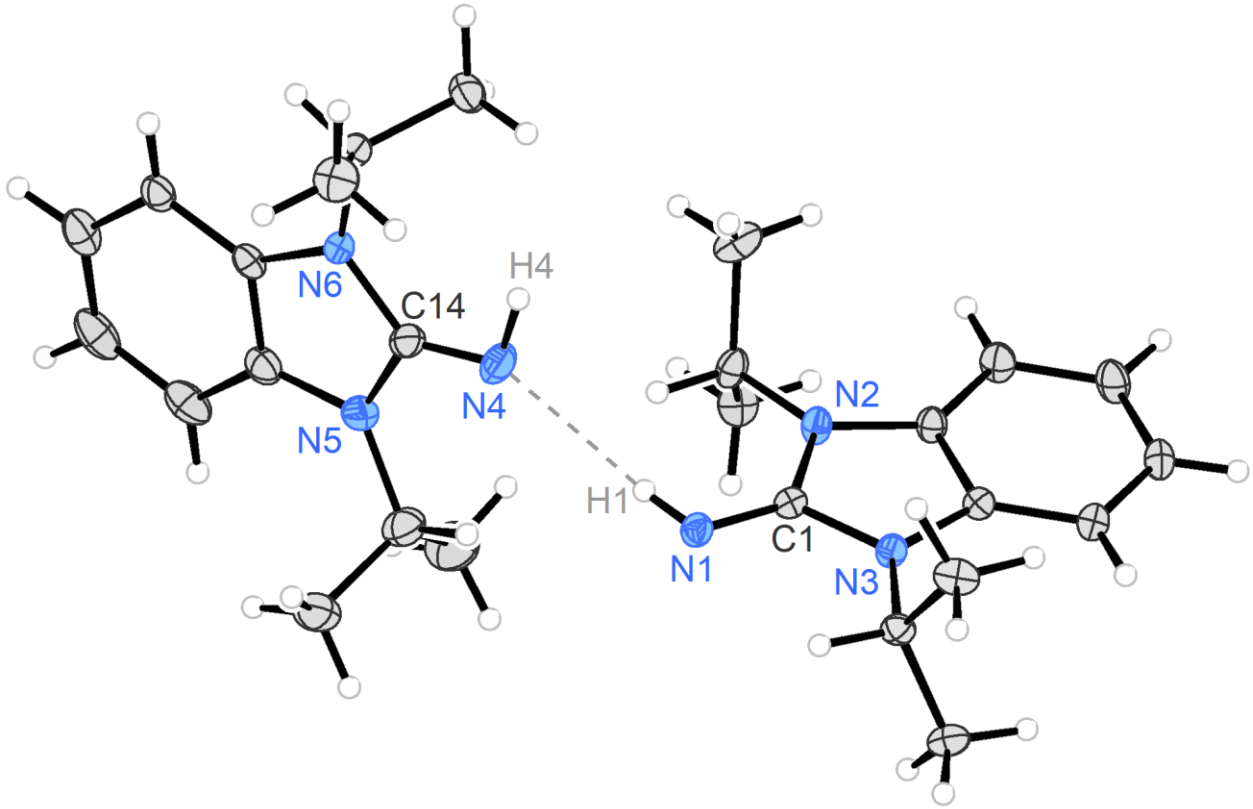


Figure S107: Molecular view of **2c** in the solid state.

Table S6. Crystal data and structure refinement for **2c**.

CCDC Number	1866032
Empirical formula	$C_{13}H_{19}N_3$
Formula weight	217.31
Temperature/K	100
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	9.9385(2)
b/Å	10.0425(2)
c/Å	24.7502(4)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2470.25(8)
Z	8

ρ_{calc}mg/mm^3	1.169
m/mm^{-1}	0.071
F(000)	944.0
Crystal size/mm^3	0.47 × 0.44 × 0.17
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection	5.224 to 59.208°
Index ranges	-13 ≤ h ≤ 13, -13 ≤ k ≤ 13, -34 ≤ l ≤ 34
Reflections collected	34800
Independent reflections	6911 [R_{int} = 0.0214, R_{sigma} = 0.0158]
Data/restraints/parameters	6911/0/305
Goodness-of-fit on F^2	1.064
Final R indexes [I>=2σ (I)]	R_1 = 0.0446, wR_2 = 0.1198
Final R indexes [all data]	R_1 = 0.0460, wR_2 = 0.1212
Largest diff. peak/hole / e Å^{-3}	0.70/-0.28
Flack parameter	0.3(3)

Single-crystal X-ray structure analysis of [3bH][BF_4]:

Single crystals were obtained by vapor diffusion of *n*-hexane into a chloroform solution of [**3b**H][BF_4]. A Single-crystal X-ray structure analysis revealed that [**3b**H][BF_4] crystallizes in the monoclinic space group $P2_1/c$. The asymmetric unit contains one molecule of [**3b**H][BF_4].

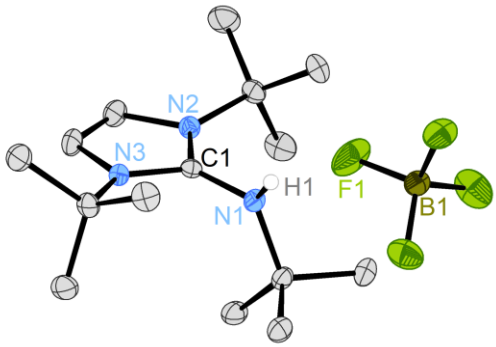


Figure S108: Molecular view of [**3b**H][BF_4] in the solid state.

Table S7. Crystal data and structure refinement for [**3b**H][BF_4].

CCDC Number	1880247
Empirical formula	$C_{15}H_{30}BF_4N_3$
Formula weight	339.23
Temperature/K	100
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	15.2506(3)
b/Å	10.8267(2)
c/Å	10.8569(2)
α/°	90
β/°	90.0900(10)
γ/°	90
Volume/Å^3	1792.62(6)
Z	4
ρ_{calc}g/cm^3	1.257
μ/mm^{-1}	0.103
F(000)	728.0
Crystal size/mm^3	0.213 × 0.104 × 0.097
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.752 to 52.738
Index ranges	-19 ≤ h ≤ 19, -13 ≤ k ≤ 13, -13 ≤ l ≤ 13
Reflections collected	24044
Independent reflections	3656 [R_{int} = 0.0407, R_{sigma} = 0.0287]
Data/restraints/parameters	3656/0/222
Goodness-of-fit on F^2	1.089
Final R indexes [I>=2σ (I)]	R_1 = 0.0416, wR_2 = 0.1067
Final R indexes [all data]	R_1 = 0.0437, wR_2 = 0.1079
Largest diff. peak/hole / e Å^{-3}	0.28/-0.20

Single-crystal X-ray structure analysis of 4e:

Single crystals were obtained by slow cooling of a saturated *n*-hexane solution of **4e** under CO_2 atmosphere. A Single-crystal X-ray structure analysis revealed that **4e** crystallizes in the monoclinic space group $P2_1/c$. The asymmetric unit contains one molecule of **4e**.

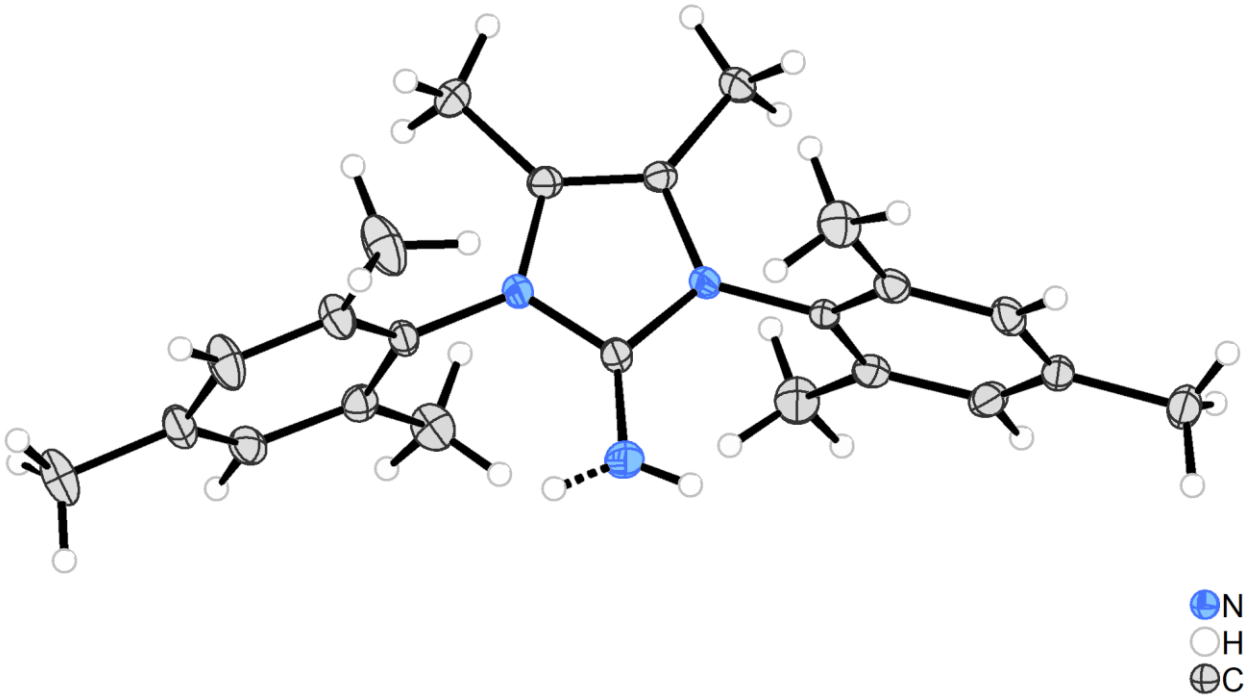


Figure S109: Molecular view of **4e** in the solid state.

Table S8. Crystal data and structure refinement for **4e**.

CCDC Number	1866036
Empirical formula	$C_{23}H_{29}N_3$
Formula weight	347.49
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	12.5296(2)
b/Å	8.09390(10)
c/Å	19.7181(4)
α/°	90
β/°	98.5378(12)
γ/°	90
Volume/Å^3	1977.52(6)
Z	4
ρ_{calc}mg/mm^3	1.167
m/mm^{-1}	0.069

F(000)	752.0
Crystal size/mm^3	0.18 × 0.17 × 0.11
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection	7.038 to 56.59°
Index ranges	$-16 \leq h \leq 16$, $-10 \leq k \leq 10$, $-26 \leq l \leq 25$
Reflections collected	22298
Independent reflections	4895 [R_{int} = 0.0407, R_{sigma} = 0.0315]
Data/restraints/parameters	4895/0/251
Goodness-of-fit on F^2	1.032
Final R indexes [I>=2σ (I)]	R_1 = 0.0499, wR_2 = 0.1284
Final R indexes [all data]	R_1 = 0.0665, wR_2 = 0.1379
Largest diff. peak/hole / e $Å^{-3}$	0.33/-0.24

Single-crystal X-ray structure analysis of 6a:

Single crystals were obtained by cooling down a hot hexane solution of **6a**. A Single-crystal X-ray structure analysis revealed that **6a** crystallizes in the monoclinic space group $P2_1/n$. The asymmetric unit contains one molecule of **6a**.

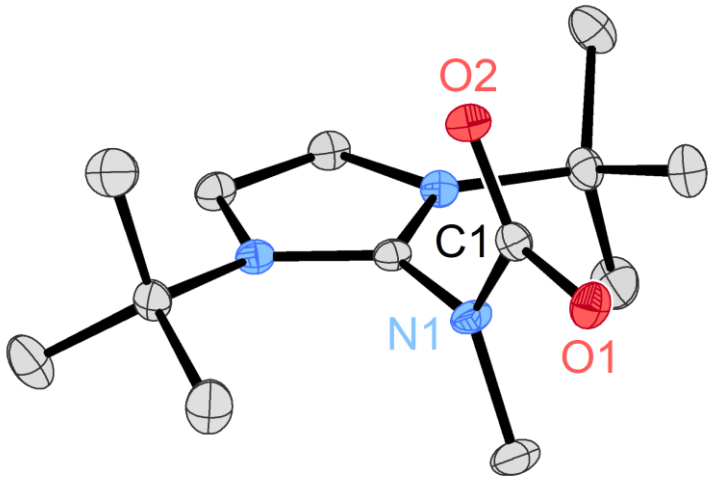


Figure S110: Molecular view of **6a** in the solid state. Hydrogen atoms are omitted.

Table S9. Crystal data and structure refinement for **6a**.

CCDC Number	1866031
Empirical formula	$C_{13}H_{23}N_3O_2$
Formula weight	253.34
Temperature/K	100
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	10.99820(10)
b/Å	9.27850(10)
c/Å	14.3717(2)
α/°	90
β/°	105.7140(10)
γ/°	90
Volume/Å^3	1411.77(3)
Z	4
ρ_{calc}g/cm^3	1.192
μ/mm^{-1}	0.082
F(000)	552.0
Crystal size/mm^3	0.321 × 0.156 × 0.056
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.164 to 56.584
Index ranges	$-14 \le h \le 14$, $-12 \le k \le 12$, $-19 \le l \le 19$
Reflections collected	14415
Independent reflections	3503 [R_{int} = 0.0300, R_{sigma} = 0.0279]
Data/restraints/parameters	3503/0/170
Goodness-of-fit on F^2	1.054
Final R indexes [I>=2σ (I)]	R_1 = 0.0398, wR_2 = 0.0956

Final R indexes [all data]	R_1 = 0.0547, wR_2 = 0.1038
Largest diff. peak/hole / e Å^{-3}	0.39/-0.23

Single-crystal X-ray structure analysis of 6b:

Single crystals were obtained by pressuring a diethylether solution of **6b** with two bar CO_2 pressure. A Single-crystal X-ray structure analysis revealed that **6b** crystallizes in the tetragonal space group $P4_1$. The asymmetric unit contains two molecules of **6b**.

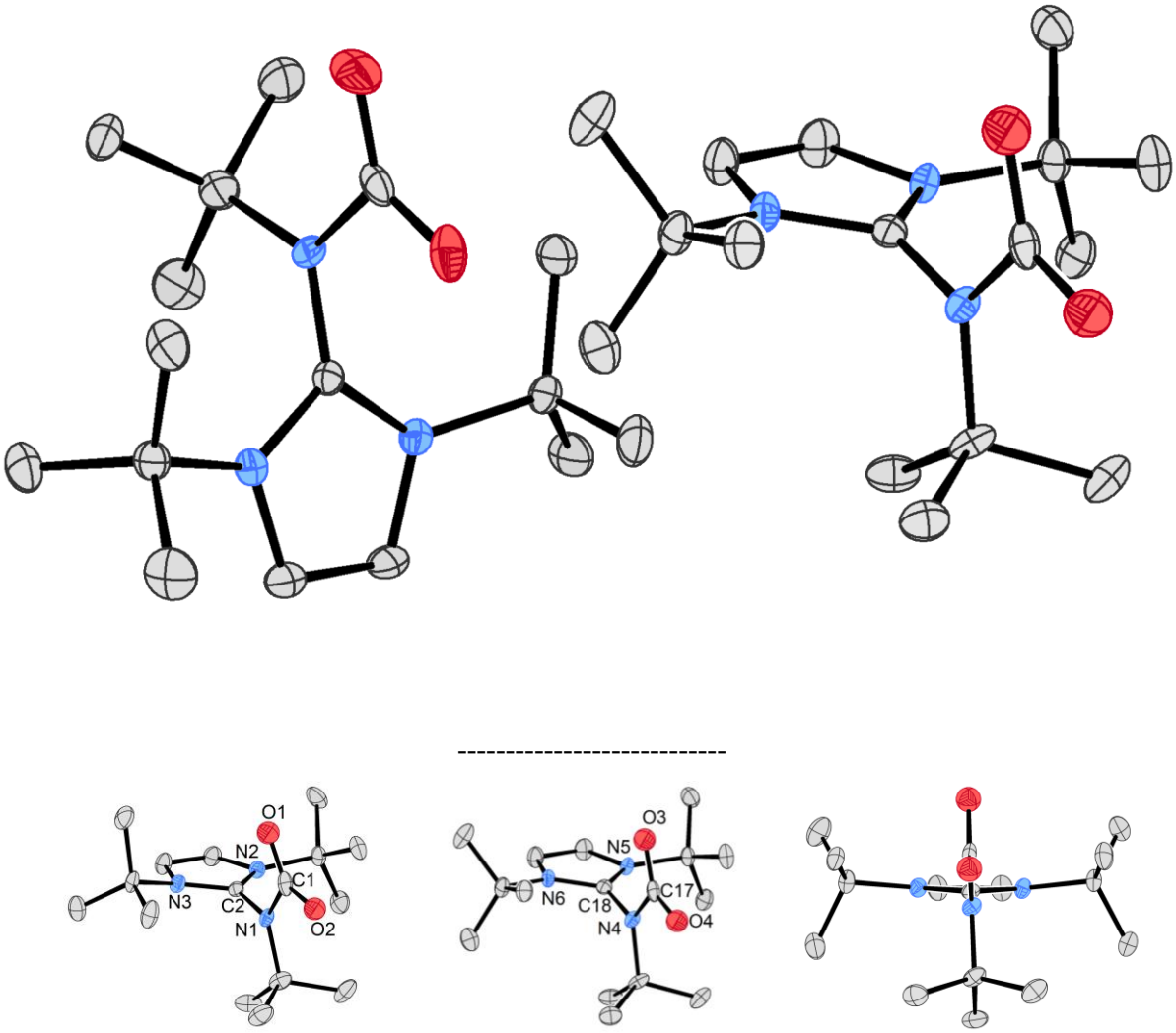


Figure S111: Molecular view of the asymmetric unit of **6b** in the solid state (top). Molecular views of the two independent molecules of **6b** (bottom). Hydrogen atoms are omitted for clarity.

Table S10. Crystal data and structure refinement for **6b**.

CCDC Number	1880248
Empirical formula	$C_{16}H_{29}N_3O_2$
Formula weight	295.42
Temperature/K	99.97

Crystal system	tetragonal
Space group	$P4_1$
a/Å	11.8565(5)
b/Å	11.8565(5)
c/Å	24.0309(13)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3378.2(3)
Z	8
ρ_{calc}g/cm^3	1.162
μ/mm^{-1}	0.077
F(000)	1296.0
Crystal size/mm^3	? × ? × ?
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	1.694 to 52.888
Index ranges	-14 ≤ h ≤ 14, -14 ≤ k ≤ 14, -29 ≤ l ≤ 30
Reflections collected	38933
Independent reflections	6906 [R_{int} = 0.0669, R_{sigma} = 0.0456]
Data/restraints/parameters	6906/1/398
Goodness-of-fit on F^2	1.072
Final R indexes [I>=2σ (I)]	R_1 = 0.0366, wR_2 = 0.0741
Final R indexes [all data]	R_1 = 0.0418, wR_2 = 0.0763
Largest diff. peak/hole / e Å^{-3}	0.14/-0.19
Flack parameter	-0.7(5)

Single-crystal X-ray structure analysis of 6c:

Single crystals were obtained by cooling down a hot hexane solution of **6c**. A Single-crystal X-ray structure analysis revealed that **6c** crystallizes in the monoclinic space group $P2_1/c$. The asymmetric unit contains four molecules of **6c** and three benzene molecules.

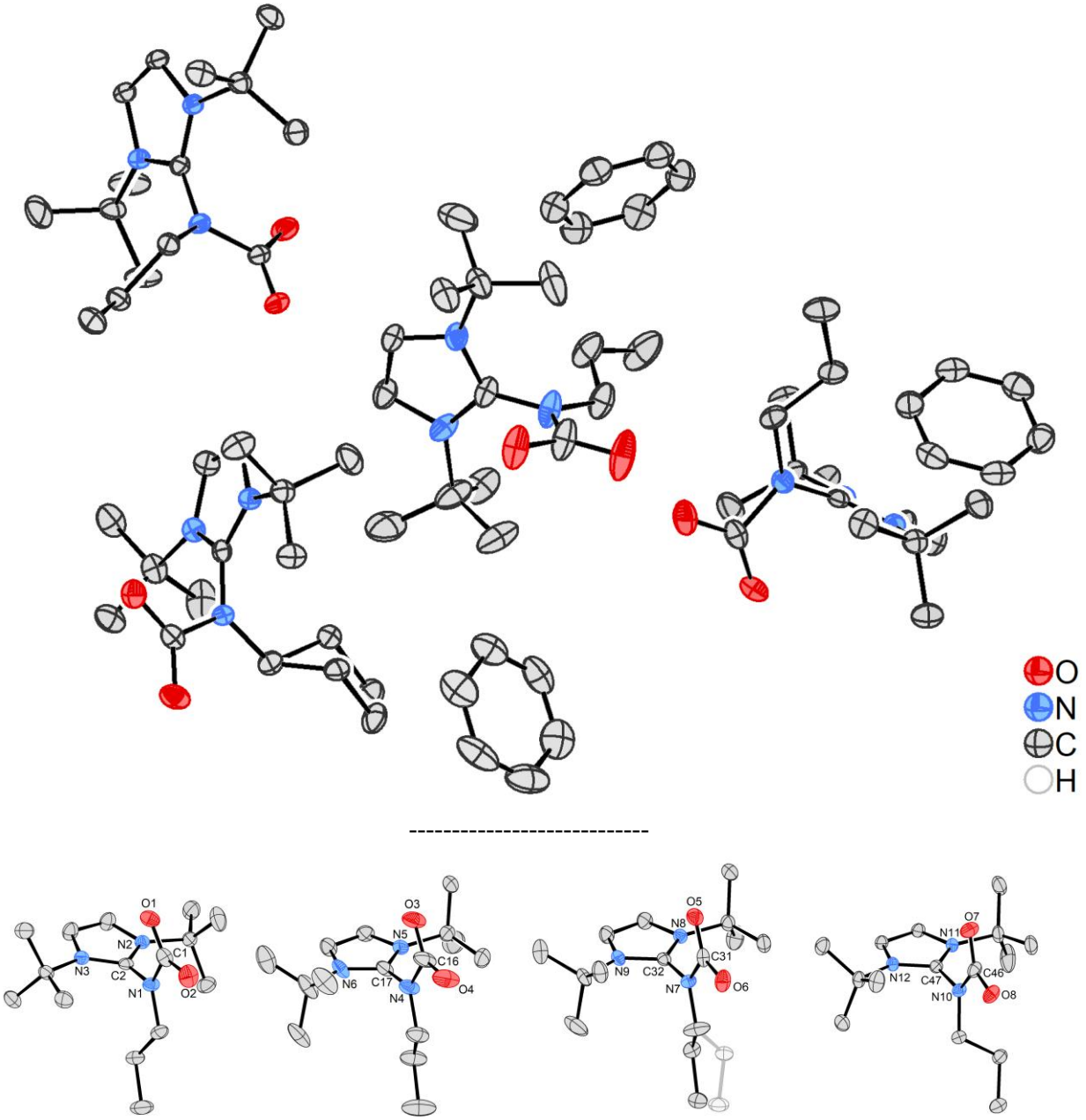


Figure S112: Molecular view of the asymmetric unit of **6c** in the solid state (top). Molecular views of the four independent molecules of **6c** (bottom). Hydrogen atoms are omitted for clarity.

Table S11. Crystal data and structure refinement for **6c**.

CCDC Number	1866038
Empirical formula	$C_{19.5}H_{31.5}N_3O_2$
Formula weight	339.98

Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	14.6071(2)
b/Å	41.9109(7)
c/Å	14.5422(2)
α/°	90
β/°	117.1590(10)
γ/°	90
Volume/Å^3	7921.1(2)
Z	16
ρ_{calc}g/cm^3	1.140
μ/mm^{-1}	0.074
F(000)	2968.0
Crystal size/mm^3	0.6 × 0.548 × 0.521
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.134 to 52.772
Index ranges	$-18 \leq h \leq 18$, $-52 \leq k \leq 52$, $-18 \leq l \leq 18$
Reflections collected	107880
Independent reflections	16183 [R_{int} = 0.0337, R_{sigma} = 0.0211]
Data/restraints/parameters	16183/0/911
Goodness-of-fit on F^2	1.046
Final R indexes [I>=2σ (I)]	R_1 = 0.0602, wR_2 = 0.1485
Final R indexes [all data]	R_1 = 0.0686, wR_2 = 0.1549
Largest diff. peak/hole / e Å^{-3}	2.25/-0.69

Single-crystal X-ray structure analysis of 7a:

Single crystals were obtained by pressuring a C_6D_6 solution of **4a** with two bar CO_2 pressure. A Single-crystal X-ray structure analysis revealed that **7a** crystallizes in the monoclinic space group *Cc*. The asymmetric unit contains one molecule of **7a**.

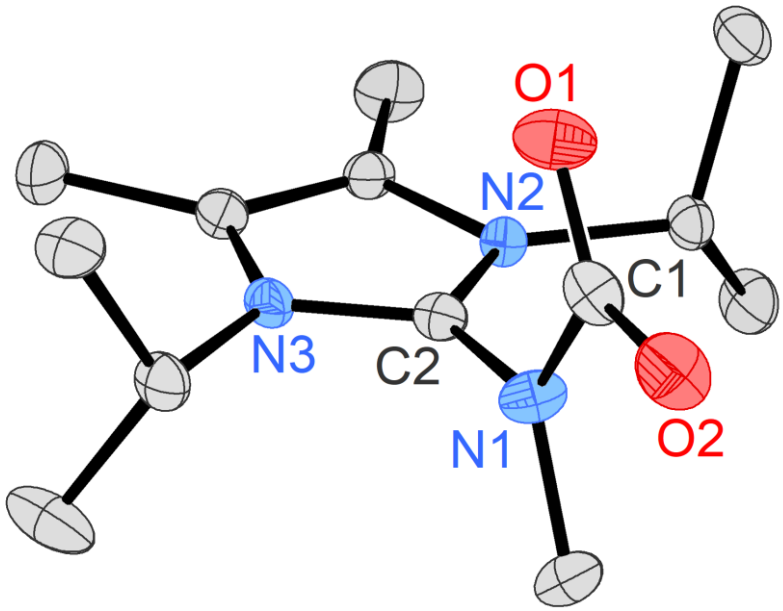


Figure S113: Molecular view of **7a** in the solid state. Hydrogen atoms are omitted.

Table S12. Crystal data and structure refinement for **7a**.

CCDC Number	1866039
Empirical formula	$C_{13}H_{23}N_3O_2$
Formula weight	253.34
Temperature/K	100(2)
Crystal system	monoclinic
Space group	*Cc*
a/Å	10.37650(10)
b/Å	13.1188(2)
c/Å	11.2806(2)
α/°	90
β/°	114.6046(6)
γ/°	90
Volume/Å^3	1396.16(4)
Z	4
ρ_{calc}mg/mm^3	1.205
m/mm^{-1}	0.082
F(000)	552.0
Crystal size/mm^3	0.52 × 0.26 × 0.23
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection	5.318 to 59.11°
Index ranges	-14 ≤ h ≤ 14, -18 ≤ k ≤ 18, -15 ≤ l ≤ 15

Reflections collected	9420
Independent reflections	3803 [R_{int} = 0.0151, R_{sigma} = 0.0188]
Data/restraints/parameters	3803/2/170
Goodness-of-fit on F^2	1.059
Final R indexes [I>=2σ (I)]	R_1 = 0.0420, wR_2 = 0.1127
Final R indexes [all data]	R_1 = 0.0426, wR_2 = 0.1135
Largest diff. peak/hole / e $Å^{-3}$	0.57/-0.18
Flack parameter	0.0(3)

Single-crystal X-ray structure analysis of 7b:

Single crystals were obtained by pressuring a C_6D_6 solution of **4b** with two bar CO_2 pressure. A Single-crystal X-ray structure analysis revealed that **7b** crystallizes in the monoclinic space group $P2_1/c$. The asymmetric unit contains one molecule of **7b**.

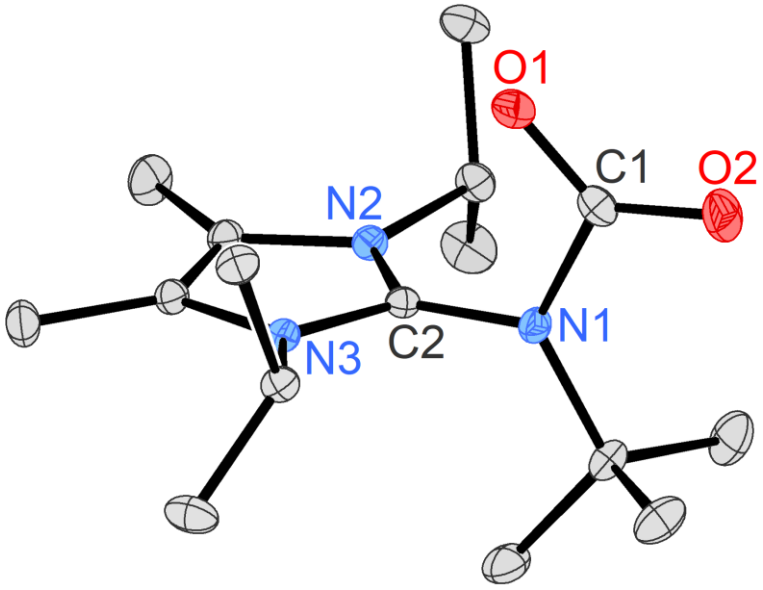


Figure S114: Molecular view of **7b** in the solid state. Hydrogen atoms are omitted.

Table S13. Crystal data and structure refinement for **7b**.

CCDC Number	1866037
Empirical formula	$C_{16}H_{29}N_3O_2$
Formula weight	295.42
Temperature/K	100
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	14.3302(2)
b/Å	9.21940(10)
c/Å	12.9756(2)
α/°	90
β/°	104.5879(6)
γ/°	90
Volume/Å^3	1659.02(4)
Z	4
ρ_{calc}mg/mm^3	1.183
m/mm^{-1}	0.079
F(000)	648.0
Crystal size/mm^3	0.58 × 0.49 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection	5.306 to 59.17°
Index ranges	-19 ≤ h ≤ 19, -12 ≤ k ≤ 12, -18 ≤ l ≤ 18
Reflections collected	27688

Independent reflections	4642 [R_{int} = 0.0183, R_{sigma} = 0.0120]
Data/restraints/parameters	4642/0/199
Goodness-of-fit on F^2	1.057
Final R indexes [I>=2σ (I)]	R_1 = 0.0368, wR_2 = 0.1011
Final R indexes [all data]	R_1 = 0.0387, wR_2 = 0.1027
Largest diff. peak/hole / e $Å^{-3}$	0.39/-0.20

Single-crystal X-ray structure analysis of 7c:

Single crystals were obtained by pressuring a hexane solution of **4c** with two bar CO_2 pressure. A Single-crystal X-ray structure analysis revealed that **7c** crystallizes in the monoclinic space group $P2_1/c$. The asymmetric unit contains one molecule of **7c**.

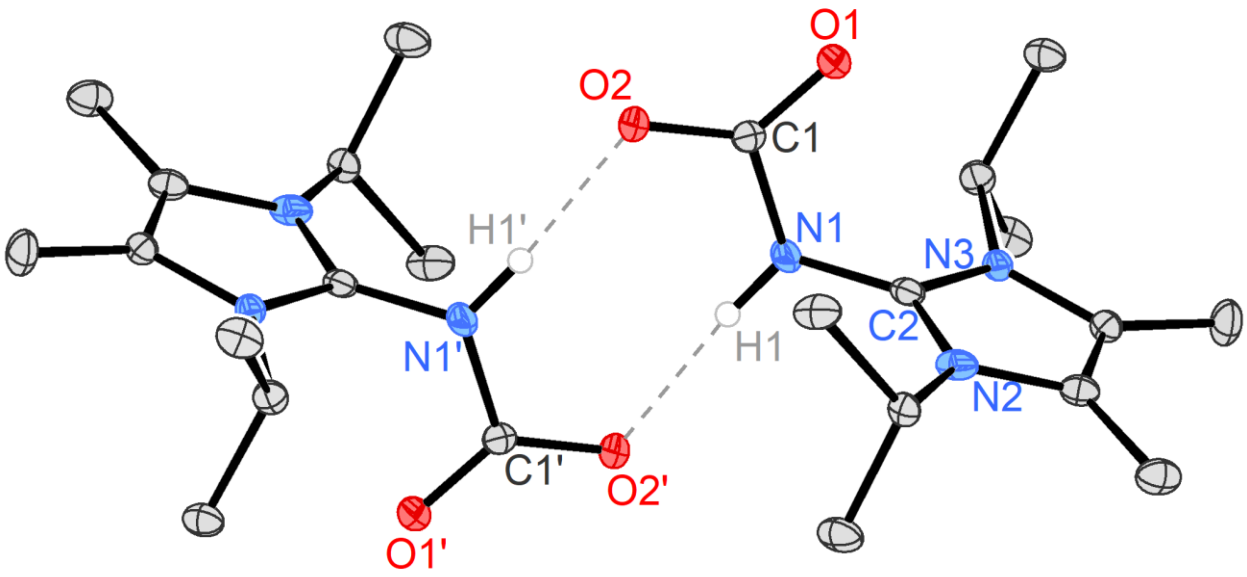


Figure S115: Molecular view of **7c** in the solid state. Hydrogen atoms except the N–H are omitted for clarity.

Table S14. Crystal data and structure refinement for **7c**.

CCDC Number	1866033
Empirical formula	$C_{12}H_{21}N_3O_2$
Formula weight	239.32
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	9.36320(10)
b/Å	18.2488(2)
c/Å	8.12900(10)
α/°	90
β/°	114.8120(7)
γ/°	90
Volume/Å^3	1260.76(3)
Z	4
ρ_{calc}mg/mm^3	1.261
m/mm^{-1}	0.087
F(000)	520.0
Crystal size/mm^3	0.28 × 0.23 × 0.11
Radiation	MoKα (λ = 0.71073)

2Θ range for data collection	6.02 to 59.11°
Index ranges	$-12 \leq h \leq 12$, $-25 \leq k \leq 25$, $-11 \leq l \leq 11$
Reflections collected	20780
Independent reflections	3523 [R_{int} = 0.0246, R_{sigma} = 0.0167]
Data/restraints/parameters	3523/0/182
Goodness-of-fit on F^2	1.096
Final R indexes [I>=2σ (I)]	R_1 = 0.0417, wR_2 = 0.1073
Final R indexes [all data]	R_1 = 0.0475, wR_2 = 0.1115
Largest diff. peak/hole / e $Å^{-3}$	0.43/-0.34

Single-crystal X-ray structure analysis of 7d:

Single crystals were obtained by pressuring a hexane solution of **4d** with two bar CO_2 pressure. A Single-crystal X-ray structure analysis revealed that **7d** crystallizes in the monoclinic space group $P2_1/c$. The asymmetric unit contains one molecule of **7d**.

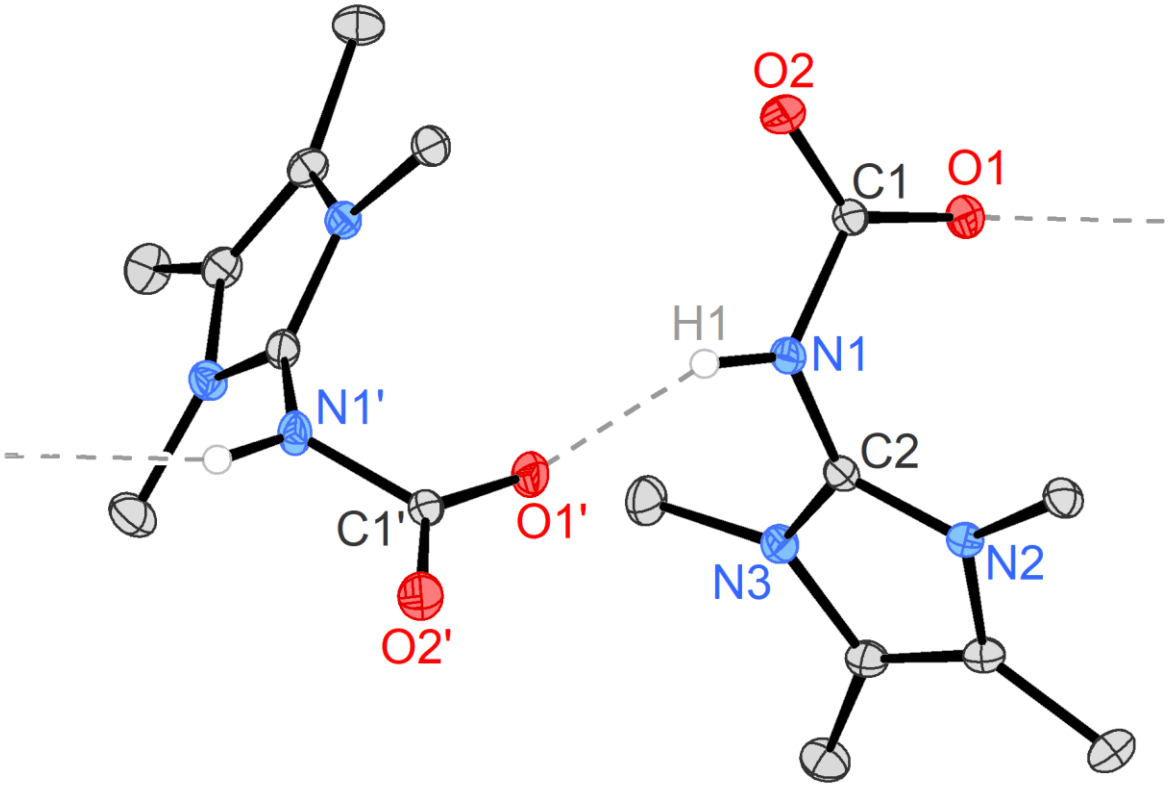


Figure S116: Molecular view of **7d** in the solid state. Hydrogen atoms except the N–H are omitted for clarity.

Table S15. Crystal data and structure refinement for **7d**.

CCDC Number	1866035
Empirical formula	$C_8H_{13}N_3O_2$
Formula weight	183.21
Temperature/K	100.01
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	6.6679(3)
b/Å	14.6889(5)
c/Å	9.6025(4)
α/°	90
β/°	104.1304(18)
γ/°	90
Volume/Å^3	912.05(6)
Z	4
ρ_{calc}mg/mm^3	1.334

m/mm^{-1}	0.098
F(000)	392.0
Crystal size/mm^3	0.12 × 0.11 × 0.08
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection	7.066 to 61.028°
Index ranges	$-8 \leq h \leq 9$, $-20 \leq k \leq 20$, $-13 \leq l \leq 13$
Reflections collected	20261
Independent reflections	2785 [R_{int} = 0.0247, R_{sigma} = 0.0139]
Data/restraints/parameters	2785/0/126
Goodness-of-fit on F^2	1.052
Final R indexes [I>=2σ (I)]	R_1 = 0.0391, wR_2 = 0.1085
Final R indexes [all data]	R_1 = 0.0416, wR_2 = 0.1110
Largest diff. peak/hole / e $Å^{-3}$	0.41/-0.34

DFT Calculations

All structures were optimized without geometry constraints using the TPSS hybrid functional[7] and an atom-pairwise dispersion correction (D3)[8,9]. A flexible triple zeta basis set (def2-TZVP)[10] was used in all calculations. In the calculations of the CO_2 binding free energy, the COSMO model[11] for implicit solvation was applied with a dielectric constant of 37.5 (CH_3CN). For the calculation of the free energy contributions (G^{RRHO}(298K)), a rotor approximation was applied for vibrational modes with wave numbers below 100 cm^{-1}.[12] The nature of all optimized stationary points was proven by the presence of no imaginary vibrational frequency. Electronic energies were recalculated with the hybrid functional PW6B95(-D3)[13] using the structures optimized with TPSS-D3. The final value for the free enthalpy ΔG(298) was obtained using the PW6B95-D3 electronic energies and G^{RRHO}(298K) from the TPSS-D3 vibrational frequencies. All calculations were performed with the TURBOMOLE 7.2 program.[14]

Binding free energies $\mathbf{\Delta G_{298}\ (CO_2)}$ were calculated from the energies in Table S1 (*solv* values) as:

$$\Delta G_{298}\ (CO_2) = [E(\mathbf{X\text{-}CO2}) - E(\mathbf{X}) - E(CO_2)] + [G^{RRHO}298(\mathbf{X\text{-}CO2}) - G^{RRHO}298(\mathbf{X}) - G^{RRHO}298(CO_2)]$$

Gas phase basicities were calculated from the vac values in Table S1 as:

$$GB = [E(\mathbf{X\text{-}H}) - E(\mathbf{X})] + [G^{RRHO}298(\mathbf{X\text{-}H}) - G^{RRHO}298(\mathbf{X})]$$

The nature of the transition structures of the isocyanate formation from the CO_2 adducts **6a** and **6b** was proven by exactly one imaginary frequency in the harmonic vibrational spectrum and IRC calculations.

Table S16. Calculated DFT Energies (E(TPSS-D3) and E(PW6B95-D3) in E_h), thermostatistical corrections for translation, rotation and vibration (G^{RRHO}298 in kcal/mol) in the gas phase (vac) and with a continuum solvation model (solv = COSMO, CH_3CN) for all molecules in the DFT study. Relative energies calculated from these values: free energies of CO_2 binding (ΔG_{298} (CO_2)) and gas phase basicity (GB) in kcal/mol. The def2-TZVP basis set was used in all calculations. ([a]: energy of transition structure relative to **3a**/**3b** and CO_2. [b]: energy of the isocyanate and the imidazolinone relative to **3a**/**3b** and CO_2.)

		E(TPSS-D3)	**G^{RRHO}298**	**E(PW6B95-D3)**	**ΔG_{298} (CO_2)**	**GB**
		[E_h]	[kcal/mol]	[E_h]	[kcal/mol]	[kcal/mol]
2a	*solv*	-710.844931	176.553	-711.596381		
2a-CO_2	*solv*	-899.558232	183.845	-900.501330	2.48	
2a	*vac*	-710.834969	177.248	-711.585971		
2a-H	*vac*	-711.248449	186.123	-711.999674		-250.73

2b	*solv*	-828.853306	225.170	-829.728059		
2b-CO_2	*solv*	-1017.572850	233.590	-1018.639809	-0.66	
2b	*vac*	-828.846308	226.190	-829.720856		
2b-H	*vac*	-829.268184	235.523	-830.143372		-255.80
2c	*solv*	-671.526377	160.663	-672.239540		
2c-CO_2	*solv*	-860.230368	167.827	-861.134233	8.79	
2c	*vac*	-671.512957	161.197	-672.225649		
2c-H	*vac*	-671.920016	169.288	-672.632484		-247.20
2x	*solv*	-553.491009	111.332	-554.077253		
2x-CO_2	*solv*	-742.202946	117.968	-742.980719	2.75	
2x	*vac*	-553.480561	110.737	-554.066428		
2x-H	*vac*	-553.888327	119.654	-554.474510		-247.16
2y	*solv*	-789.495795	210.985	-790.329466		
2y-CO_2	*solv*	-978.214968	219.291	-979.239707	0.17	
2y	*vac*	-789.487948	210.625	-790.321336		
2y-H	*vac*	-789.904482	220.170	-790.736821		-251.18
3a	*solv*	-635.749539	182.717	-636.412754		
3a-CO_2	*solv*	-824.482763	190.357	-825.338505	-10.23	
3a-CO2-TS	*solv*	-824.42750725	188.451501	-825.27921428	+25.07[a]	
Me-NCO	*solv*	-208.11940669	14.625567	-208.32978167	-20.16[b]	
Imidazolinone	*solv*	-616.35619658	160.305017	-616.99997365		
3a	*vac*	-635.742208	183.502	-636.405149		
3a-H	*vac*	-636.172210	192.258	-636.834591		-260.72
3b	*solv*	-753.754039	231.462	-754.541012		
3b-CO_2	*solv*	-942.485307	240.453	-943.464434	-7.41	
3b-CO2-TS	*solv*	-942.44483185	239.739460	-943.42180910	+18.62[a]	
tBu-NCO	*solv*	-943.42180910	239.739460	-943.42180910	-31.56[b]	
3b	*vac*	-753.748163	232.201	-754.534955		
3b-H	*vac*	-754.180736	241.984	-754.966988		-261.32
3c	*solv*	-714.423721	215.590	-715.169484		
3c-CO_2	*solv*	-903.158399	225.243	-904.097686	-9.75	
3c	*vac*	-714.416211	216.573	-715.161592		
3c-H	*vac*	-714.848057	225.757	-715.594355		-262.38
3d	*solv*	-911.109058	297.652	-912.062168		
3d-CO_2	*solv*	-1099.843819	307.686	-1100.990303	-9.33	
3d	*vac*	-911.100886	298.703	-912.053641		

3d-H	*vac*	-911.534190	308.305	-912.487645		-262.74
3x	*solv*	-399.735186	83.186	-400.150292		
3x-CO_2	*solv*	-588.457998	91.926	-589.064873	-2.12	
3x	*vac*	-399.723602	83.343	-400.138240		
3x-H	*vac*	-400.139365	92.651	-400.554288		-251.77
3y	*solv*	-557.092372	149.388	-557.673183		
3y-CO_2	*solv*	-745.817556	157.643	-746.589236	-3.53	
3y	*vac*	-557.082532	150.077	-557.663254		
3y-H	*vac*	-557.503887	159.279	-558.084822		-255.34
4a	*solv*	-635.771559	182.177	-636.434988		
4a-CO_2	*solv*	-824.500970	188.944	-825.355476	-7.80	
4a	*vac*	-635.762138	182.869	-636.425143		
4a-H	*vac*	-636.190500	191.436	-636.852958		-259.89
4b	*solv*	-753.781515	230.904	-754.568792		
4b-CO_2	*solv*	-942.515269	238.766	-943.494308	-9.86	
4b	*vac*	-753.773891	231.777	-754.560770		
4b-H	*vac*	-754.211414	240.842	-754.998984		-265.92
4c	*solv*	-596.453179	165.693	-597.077860		
4c-CO_2	*solv*	-785.170902	172.873	-785.987004	-0.26	
4c	*vac*	-596.439468	166.379	-597.063651		
4c-H	*vac*	-596.860648	175.148	-597.484916		-255.58
4d	*solv*	-439.102223	100.068	-439.562216		
4d-CO_2	*solv*	-627.819223	108.040	-628.470060	1.34	
4d	*vac*	-439.087556	99.338	-439.546948		
4d-H	*vac*	-439.504303	108.077	-439.963617		-252.72
4x	*solv*	-478.420927	115.074	-478.919222		
4x-CO_2	*solv*	-667.147349	122.305	-667.837317	-5.83	
4x	*vac*	-478.409999	115.816	-478.907663		
4x-H	*vac*	-478.833650	124.963	-479.331250		-256.66
4y	*solv*	-714.422870	215.383	-715.168866		
4y-CO_2	*solv*	-903.153574	223.838	-904.090759	-6.99	
4y	*vac*	-714.416467	216.205	-715.162181		
4y-H	*vac*	-714.842898	225.470	-715.586949		-257.28
5a	*solv*	-636.967297	197.551	-637.630602		
5a-CO_2	*solv*	-825.682267	205.940	-826.535514	3.60	

5a	*vac*	-636.960705	198.215	-637.623857		
5a-H	*vac*	-637.378630	206.942	-638.038789		-251.65
5x	*solv*	-400.950736	98.480	-401.364494		
5x-CO_2	*solv*	-589.664082	105.015	-590.268657	2.22	
5x	*vac*	-400.940862	98.824	-401.354437		
5x-H	*vac*	-401.353162	107.291	-401.765692		-249.60
5y	*solv*	-558.306589	164.585	-558.886910		
5y-CO_2	*solv*	-747.020914	170.981	-747.791015	2.11	
5y	*vac*	-558.297562	165.084	-558.877664		
5y-H	*vac*	-558.715856	174.023	-559.294469		-252.61
MTBD	*solv*	-478.426796	121.046	-478.927026		
MTBD-CO_2	*solv*	-667.142689	129.074	-667.832424	2.93	
MTDB	*vac*	-478.416603	121.352	-478.916647		
MTDB-H	*vac*	-478.839385	130.367	-479.338844		-255.92
DBU	*solv*	-462.381519	129.625	-462.867647		
DBU-CO_2	*solv*	-651.092056	136.496	-651.767225	5.43	
DBU	*vac*	-462.371031	129.824	-462.857049		
DBU-H	*vac*	-462.789176	139.179	-463.273963		-252.26
DBN	*solv*	-383.710764	95.200	-384.114657		
DBN-CO_2	*solv*	-572.427210	102.287	-573.020937	1.44	
DBN	*vac*	-383.700061	95.380	-384.103823		
DBN-H	*vac*	-384.113639	104.682	-384.516268		-249.51
TBD	*solv*	-439.098368	105.343	-439.559310		
TBD-CO_2	*solv*	-627.824526	112.338	-628.474195	-4.05	
TBD	*vac*	-439.085145	105.663	-439.545894		
TBD-H	*vac*	-439.505584	114.146	-439.966018		-255.15
CO_2	*solv*	-188.698584	-6.276	-188.887279		

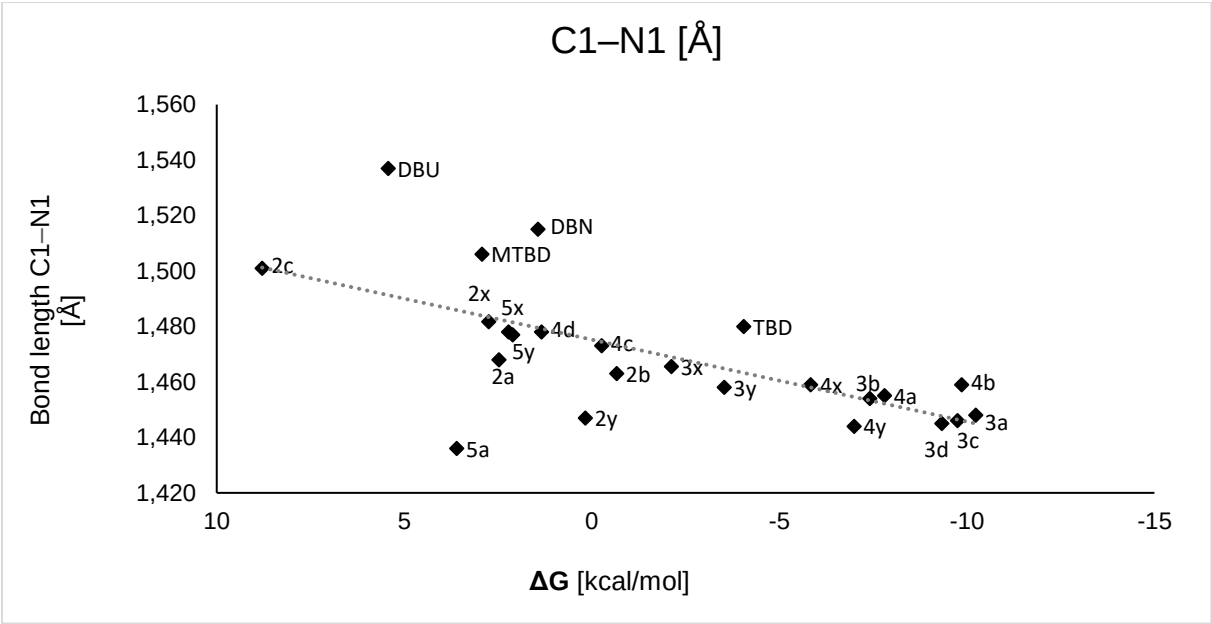


Figure S117: Calculated CO_2 binding energies (kcal/mol) vs. calculated C1–N1 bond lengths (Å).

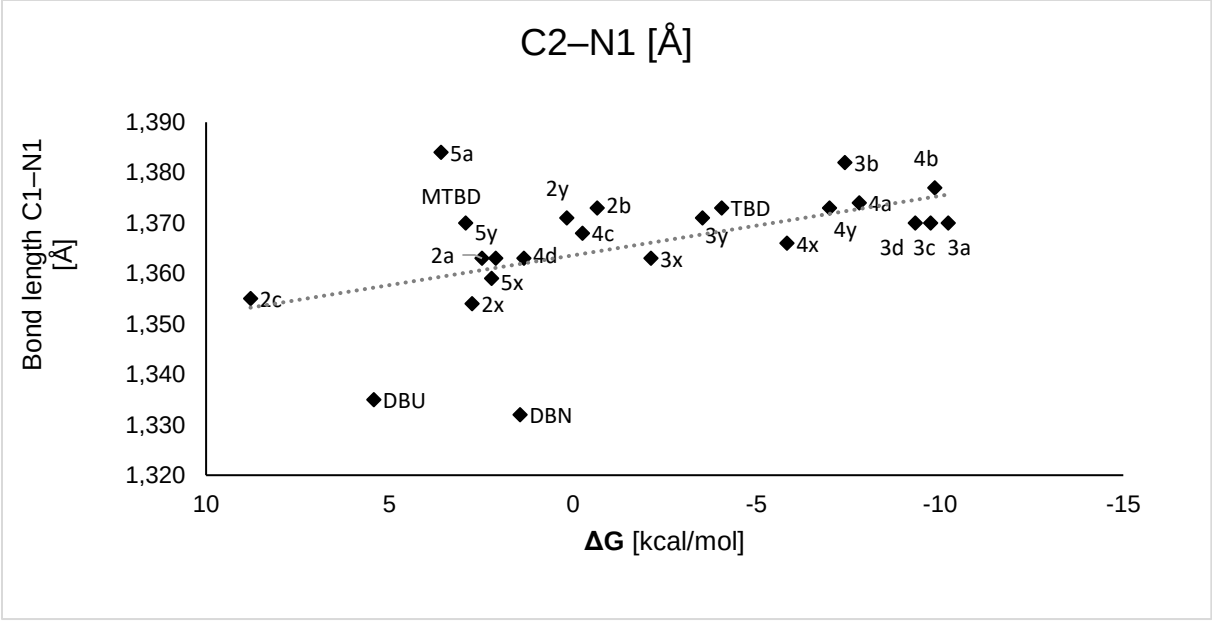


Figure S118: Calculated CO_2 binding energies (kcal/mol) vs. calculated C2–N1 bond lengths (Å).

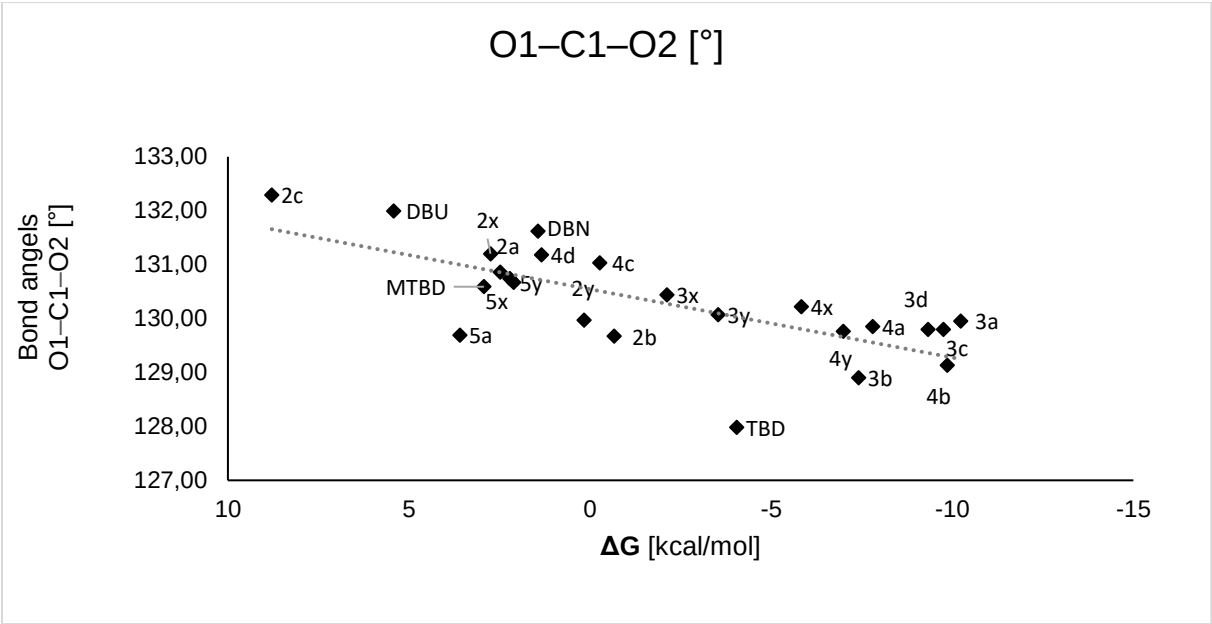


Figure S119: Calculated CO_2 binding energies (kcal/mol) vs. calculated O1–C1–O2 bond angles (°).

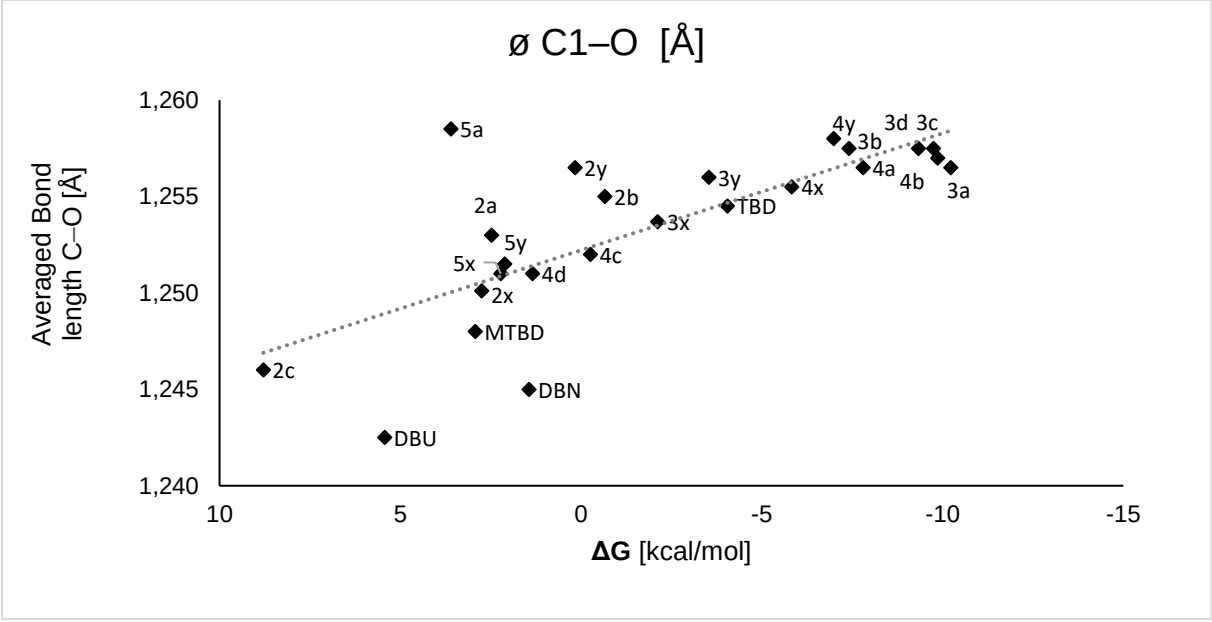
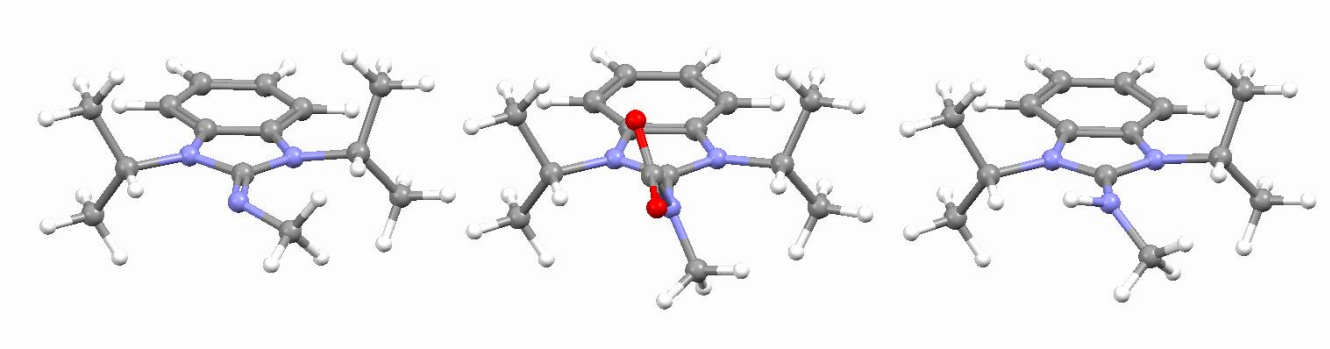
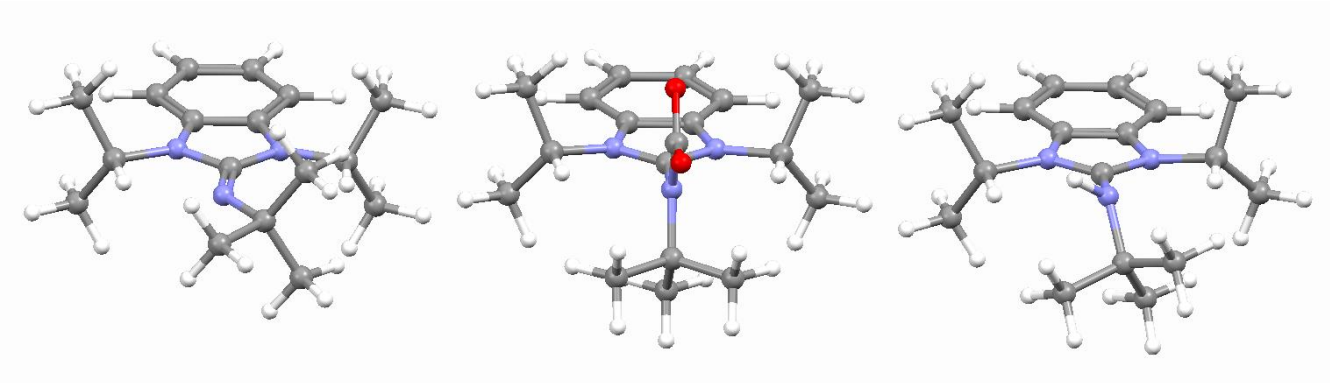


Figure S120: Calculated CO_2 binding energies (kcal/mol) vs. calculated average C1–O bond lengths (Å).

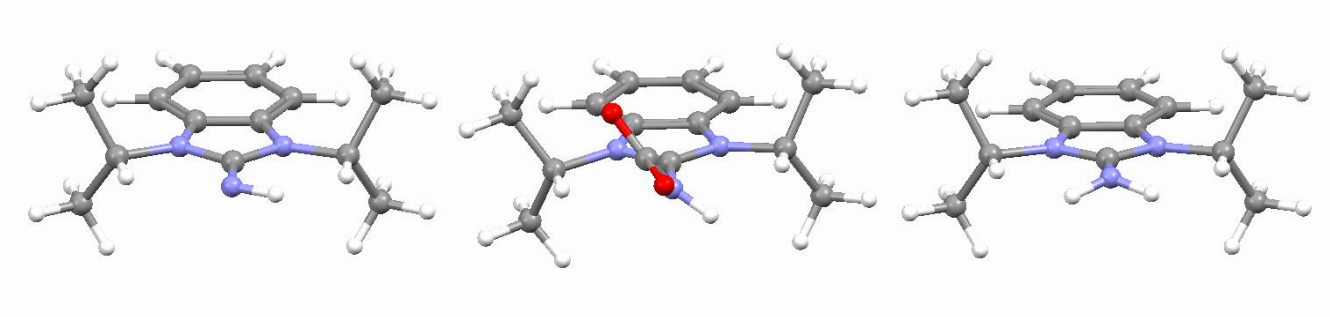
Figure S121. Optimized molecular structures of the imines investigated in the DFT calculations, the CO_2 adduct of the imines (solution structures), and the protonated imines.



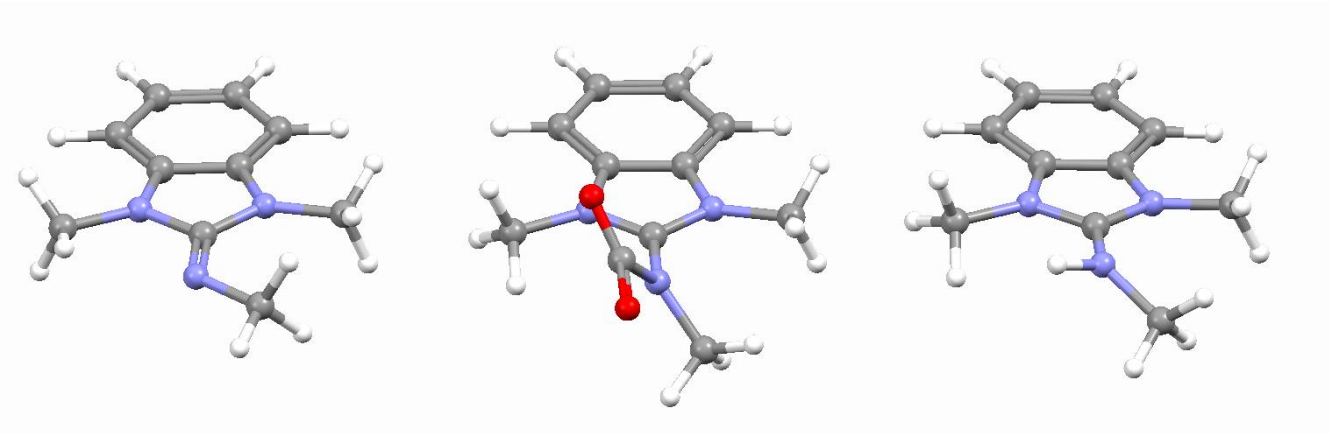
(a) **2a** (left), **2a-CO_2** (center), **2a-H** (right)



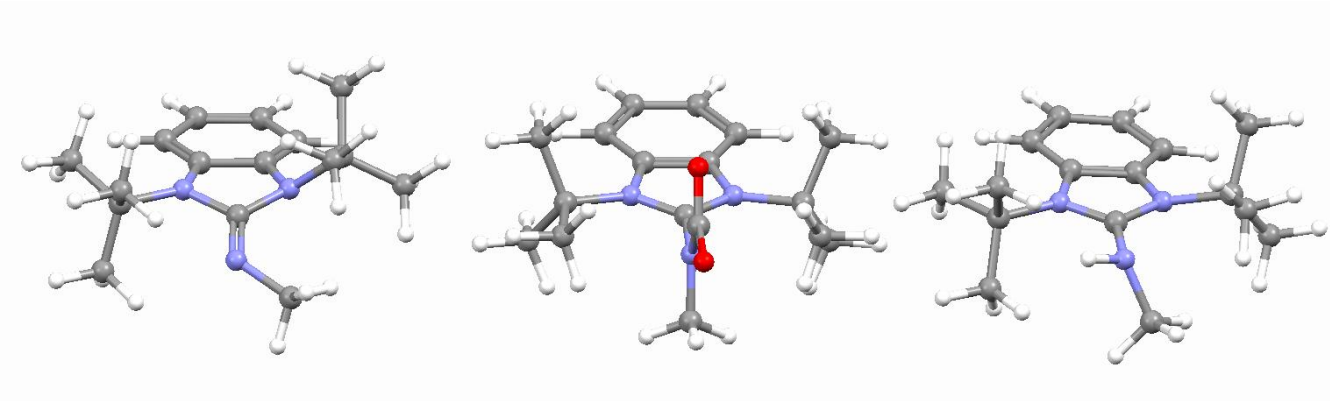
(b) **2b** (left), **2b-CO_2** (center), **2b-H** (right)



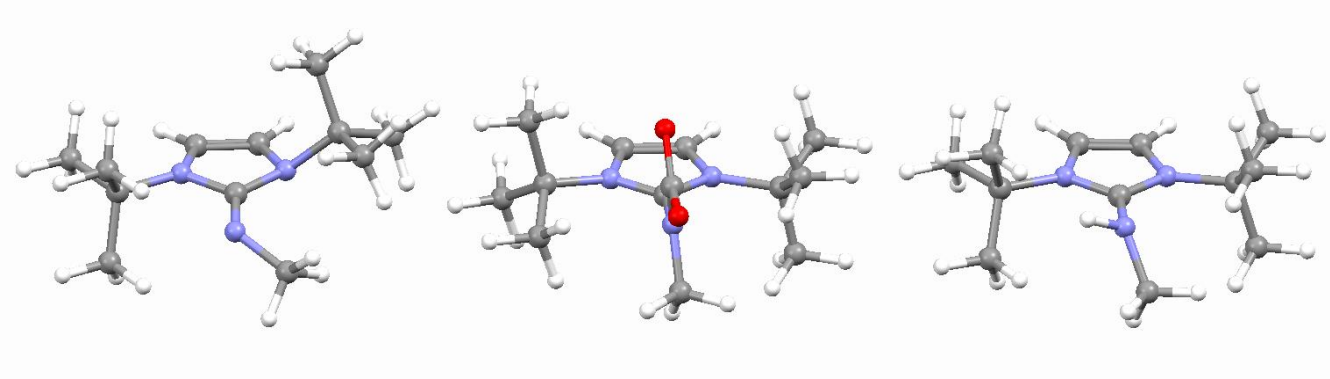
(c) **2c** (left), **2c-CO_2** (center), **2c-H** (right)



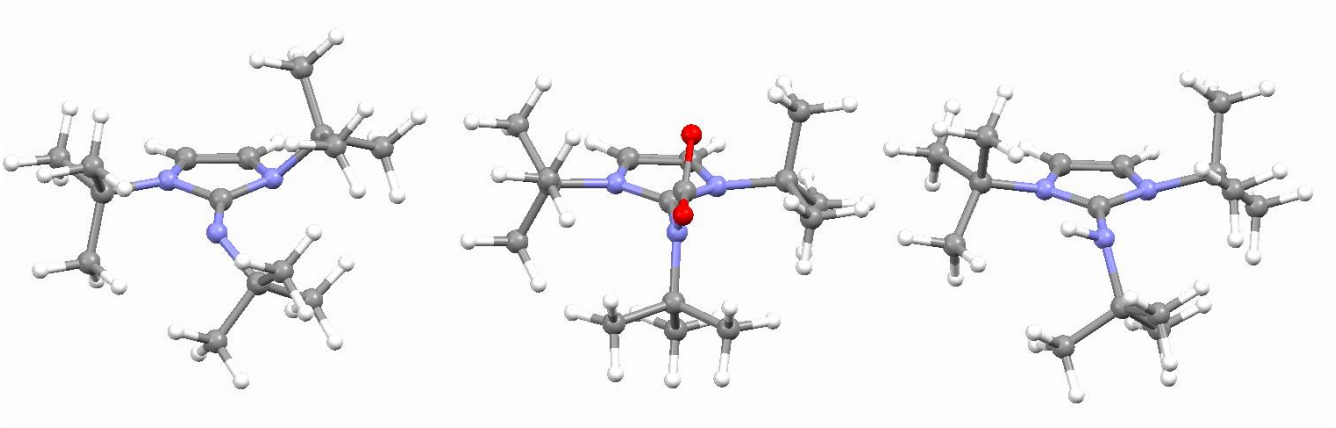
(d) **2x** (left), **2x-CO_2** (center), **2x-H** (right)



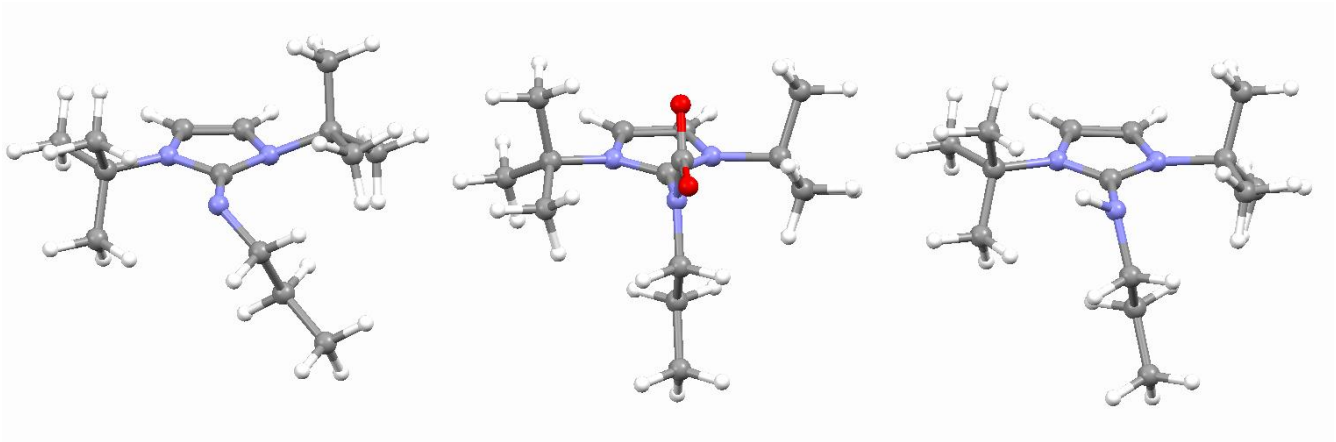
(e) **2y** (left), **2y-CO_2** (center), **2y-H** (right)



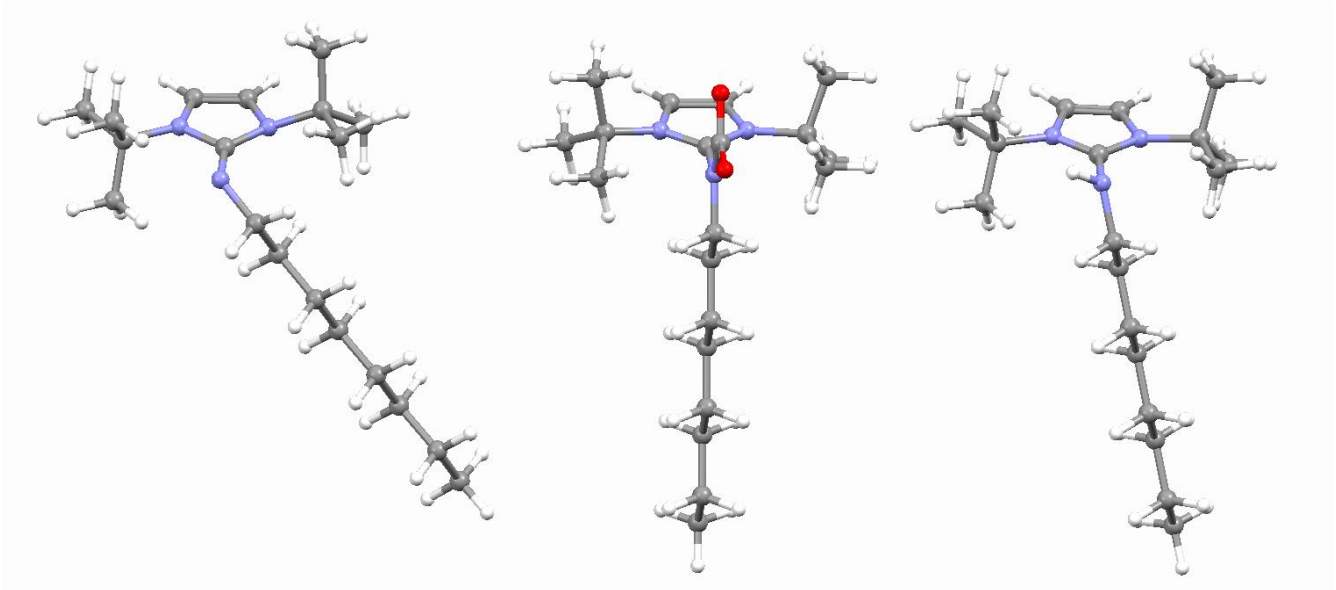
(f) **3a** (left), **3a-CO_2** (center), **3a-H** (right)



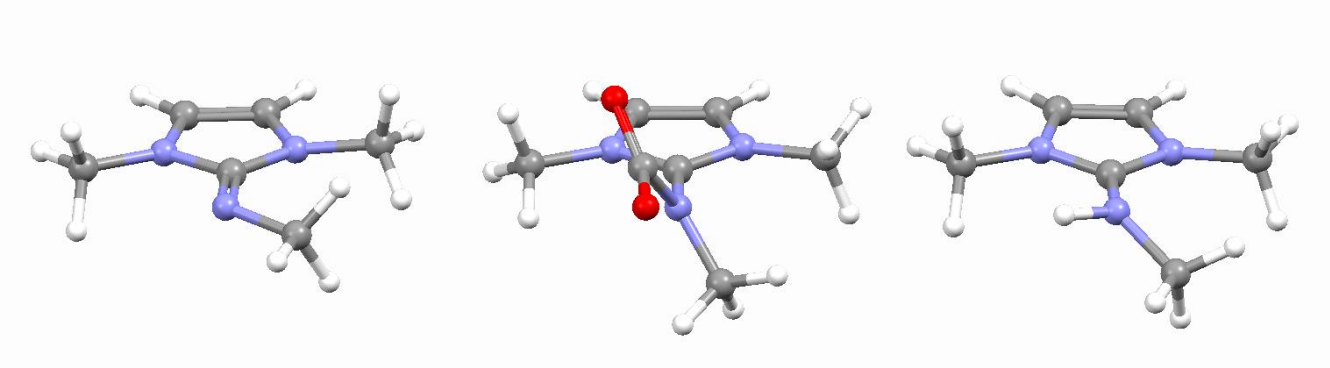
(g) **3b** (left), **3b-CO_2** (center), **3b-H** (right)



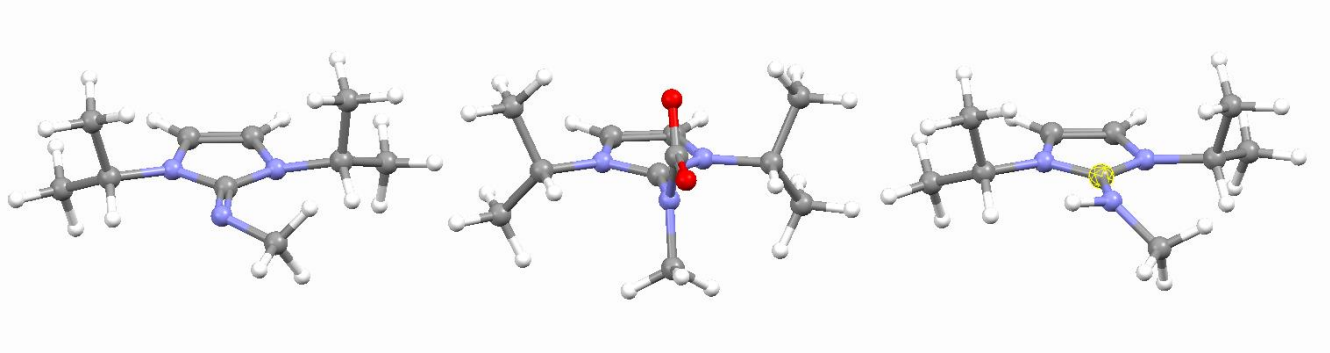
(h) **3c** (left), **3c-CO_2** (center), **3c-H** (right)



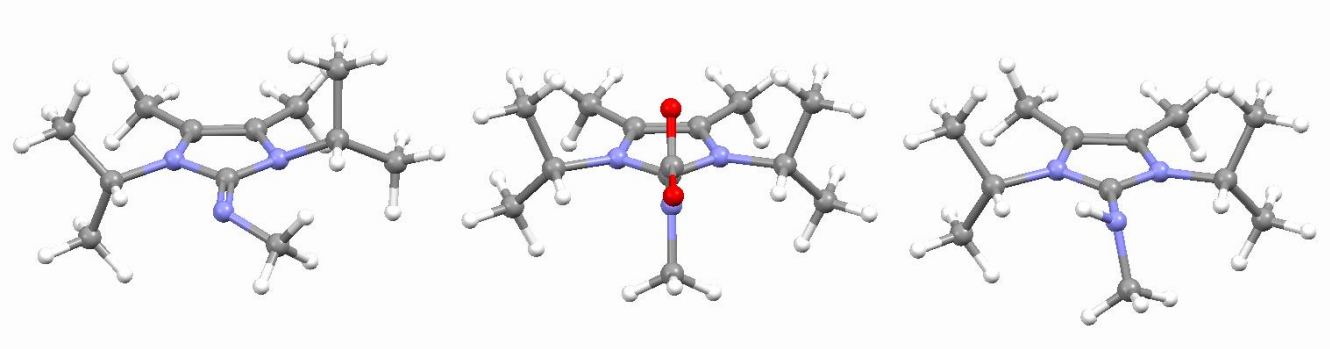
(i) **3d** (left), **3d-CO_2** (center), **3d-H** (right)



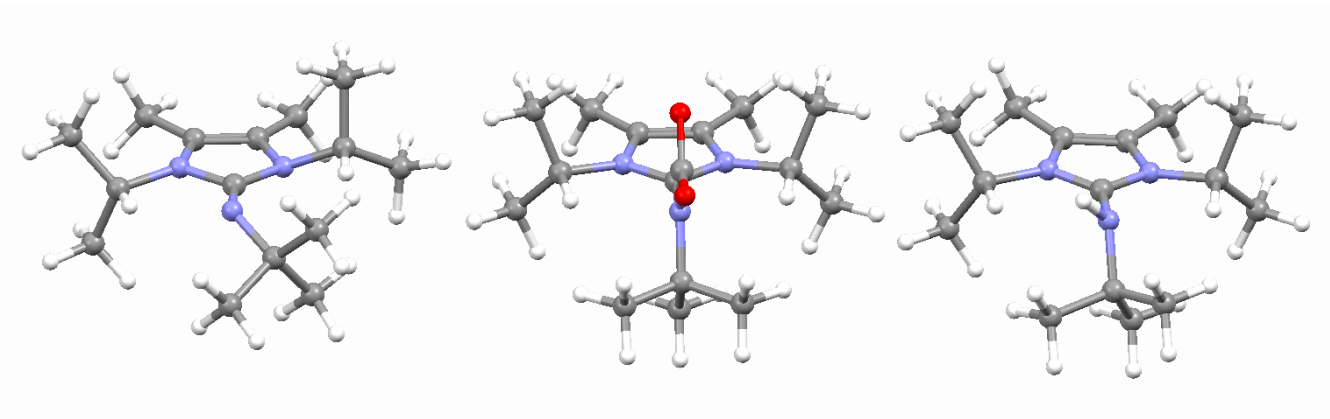
(j) **3x** (left), **3x-CO_2** (center), **3x-H** (right)



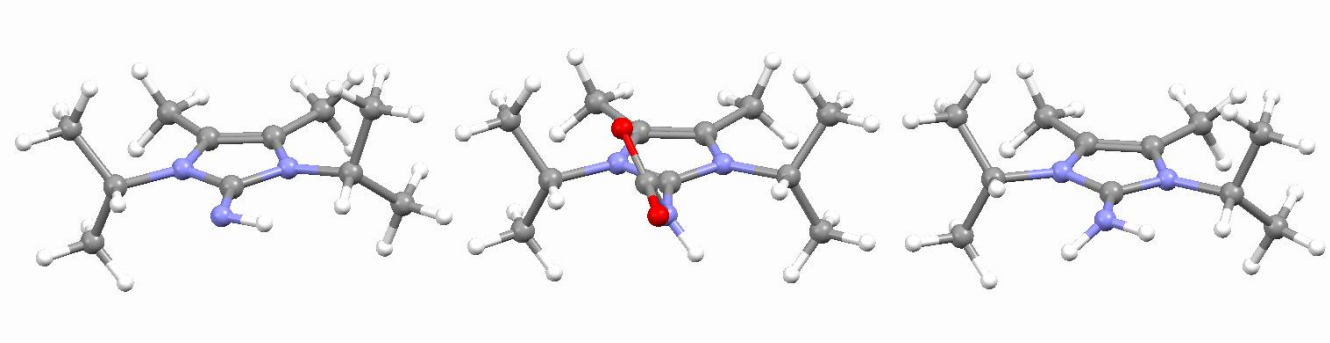
(k) **3y** (left), **3y-CO_2** (center), **3y-H** (right)



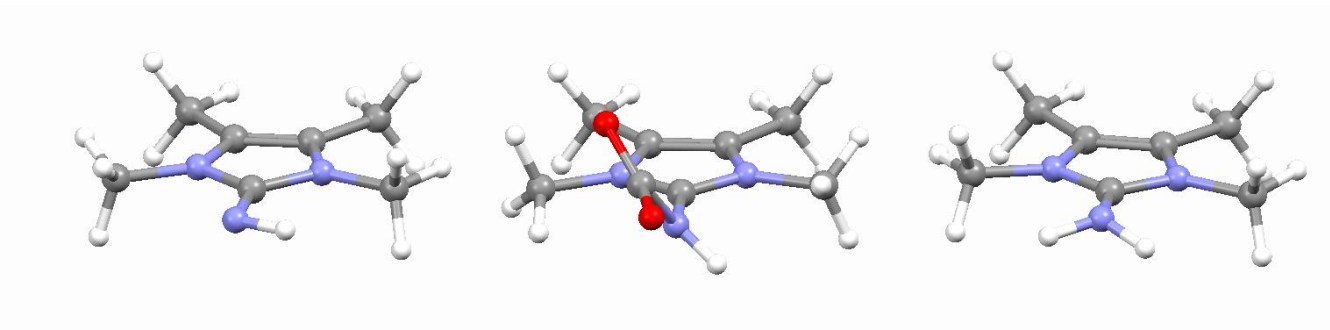
(l) **4a** (left), **4a-CO_2** (center), **4a-H** (right)



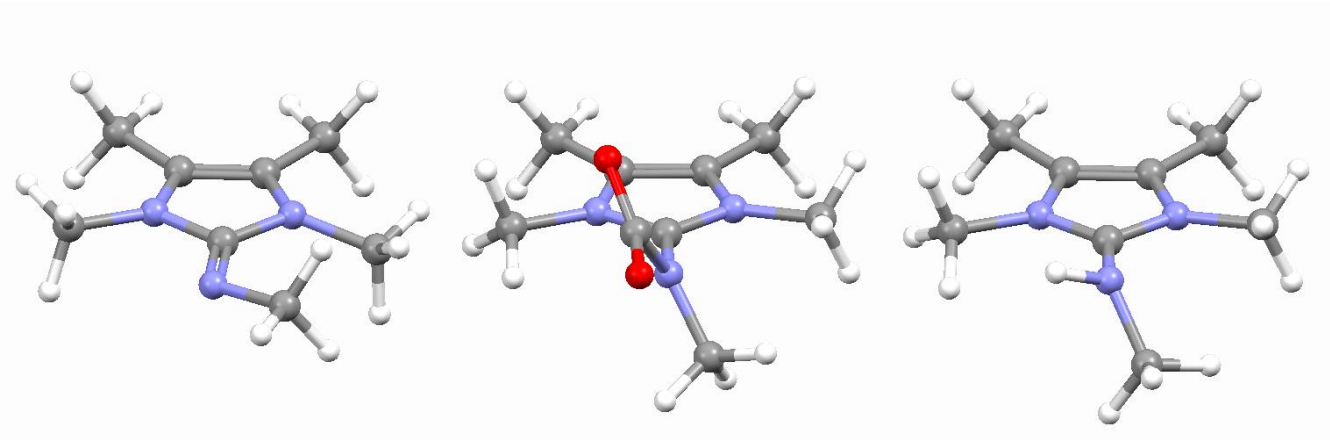
(m) **4b** (left), **4b-CO_2** (center), **4b-H** (right)



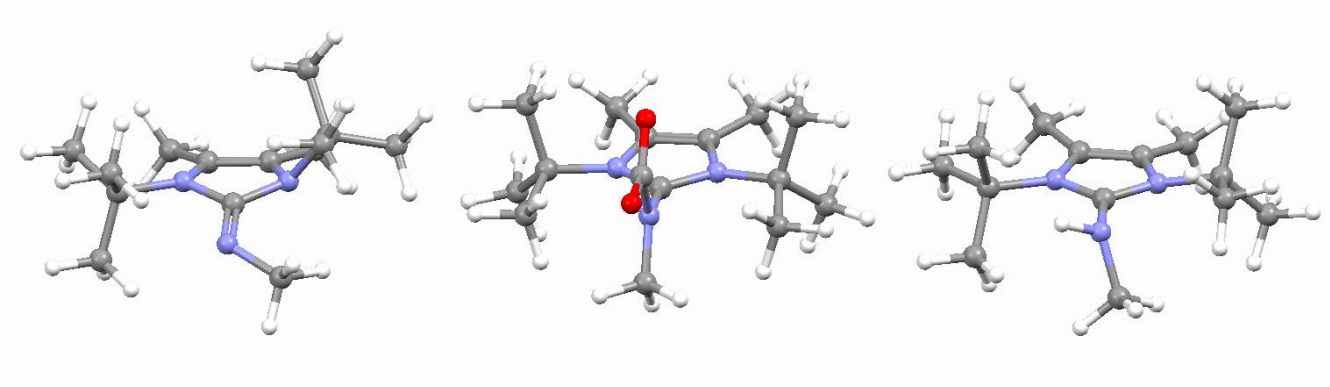
(n) **4c** (left), **4c-CO_2** (center), **4c-H** (right)



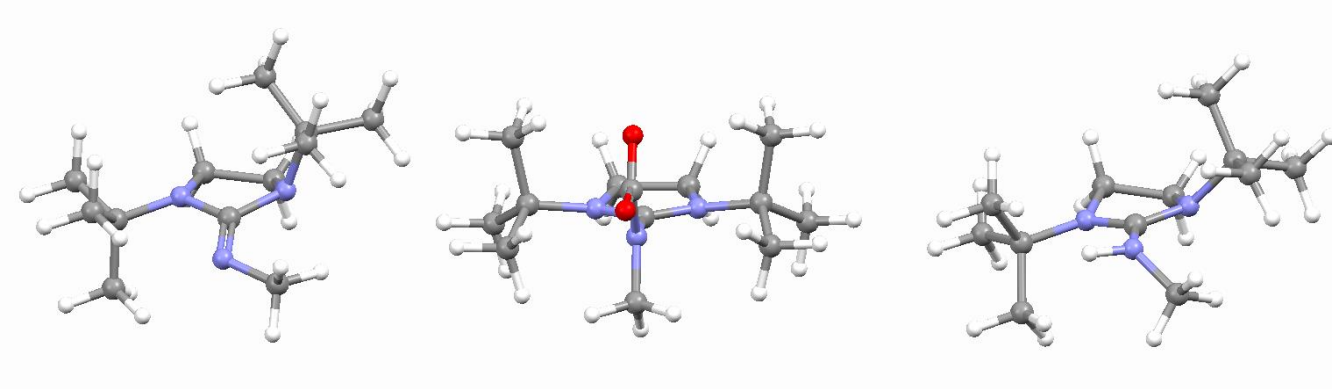
(o) **4d** (left), **4d-CO_2** (center), **4d-H** (right)



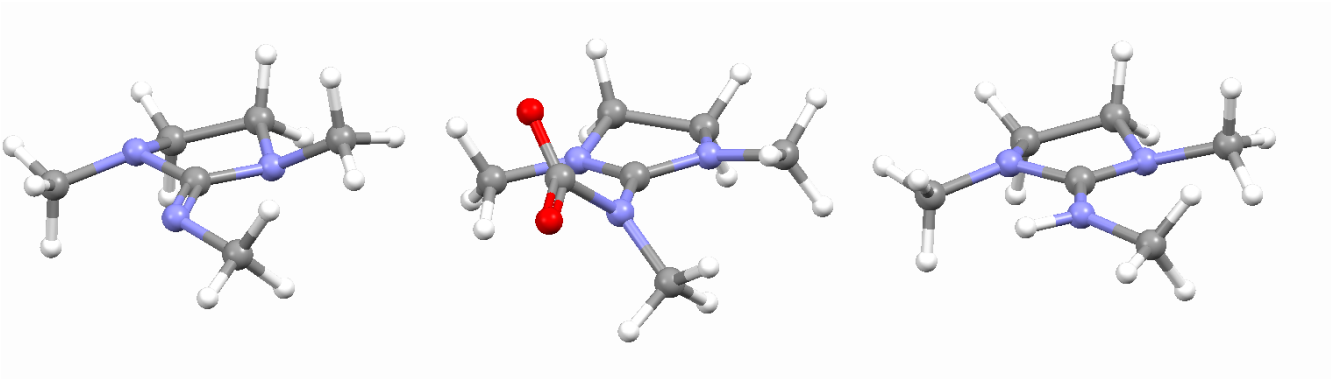
(q) **4x** (left), **4x-CO_2** (center), **4x-H** (right)



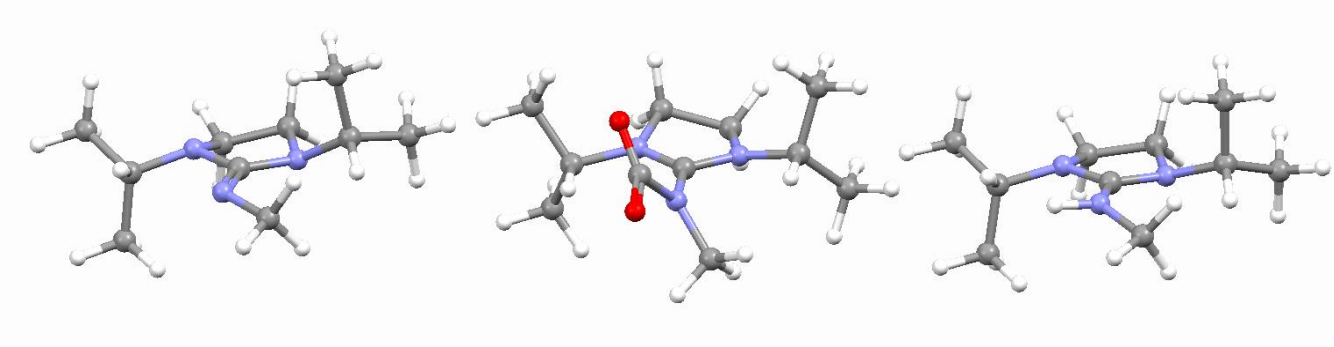
(r) **4y** (left), **4y-CO_2** (center), **4y-H** (right)



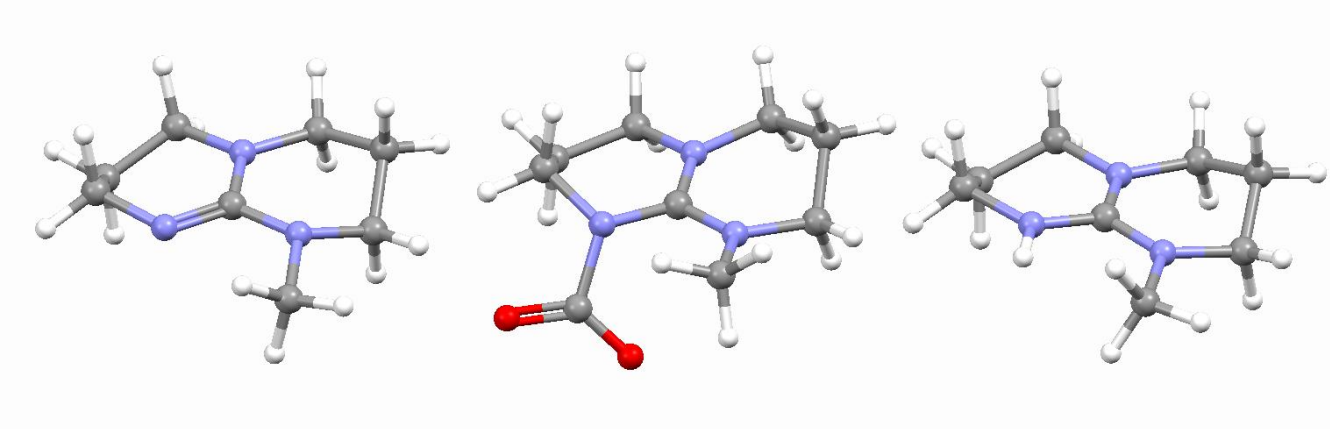
(s) **5a** (left), **5a-CO_2** (center), **5a-H** (right)



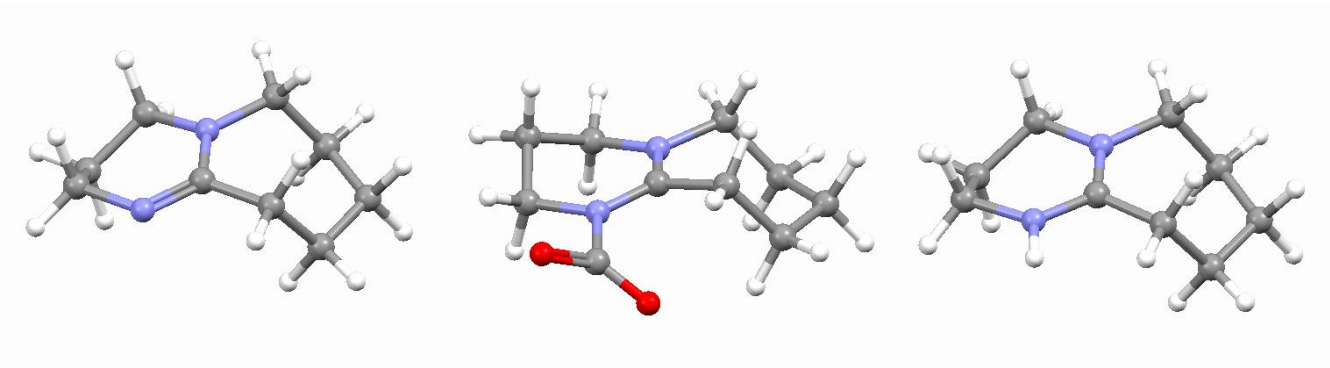
(t) **5x** (left), **5x-CO_2** (center), **5x-H** (right)



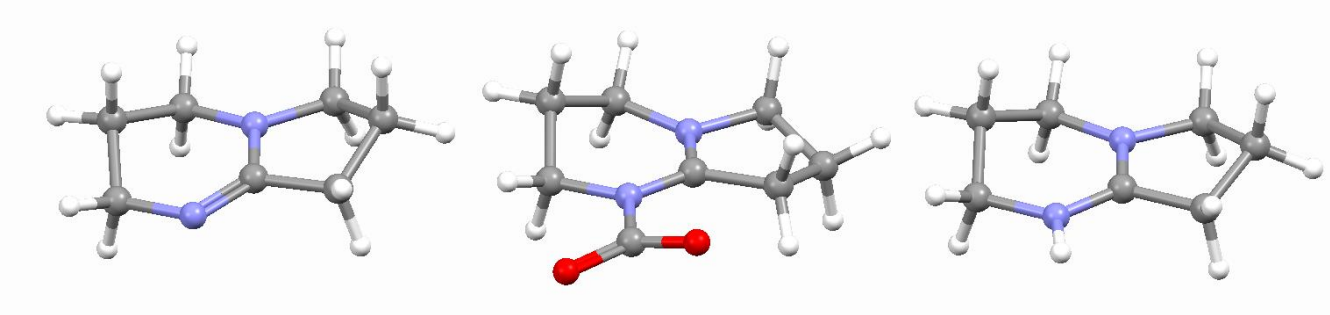
(u) **5y** (left), **5y-CO_2** (center), **5y-H** (right)



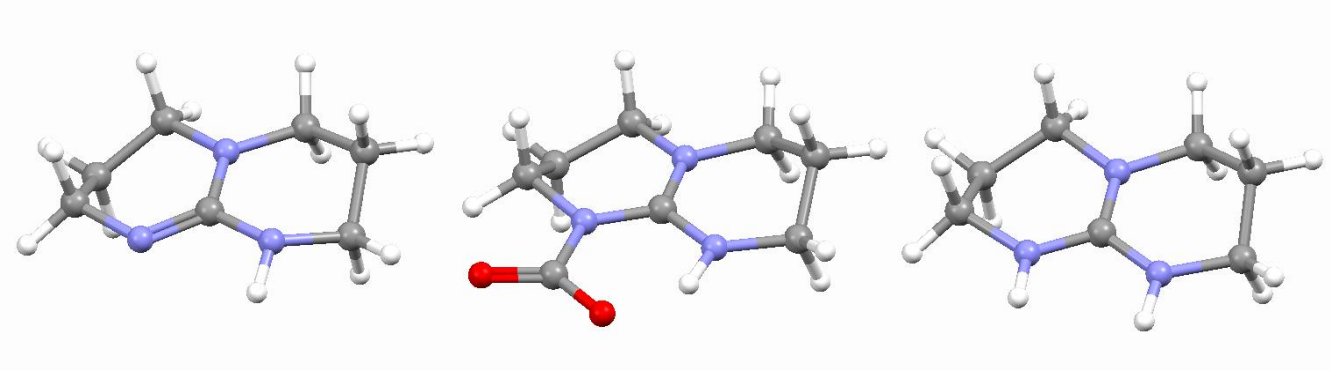
(v) **MTBD** (left), **MTBD-CO_2** (center), **MTBD-H** (right)



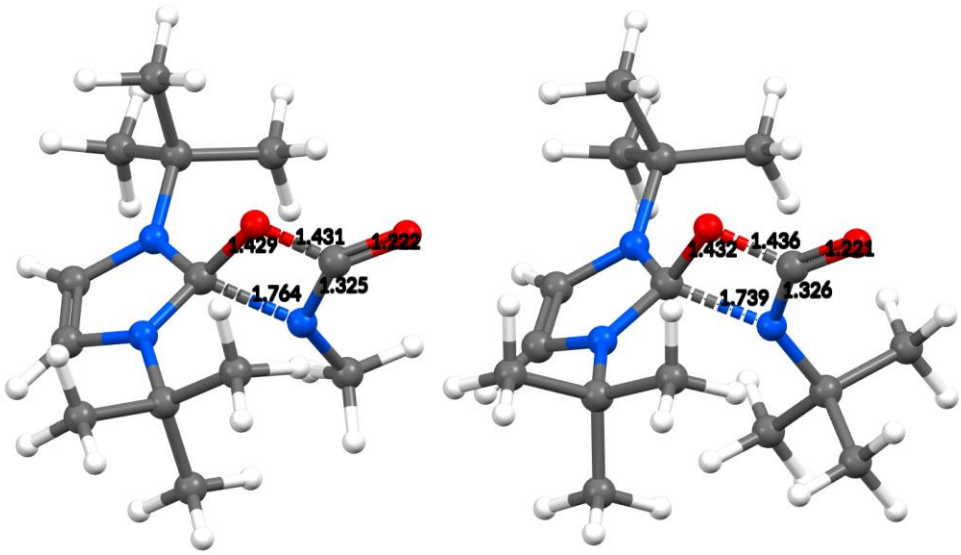
(w) **DBU** (left), **DBU-CO_2** (center), **DBU-H** (right)



(x) **DBN** (left), **DBN-CO_2** (center), **DBN-H** (right)



(y) **TBD** (left), **TBD-CO_2** (center), **TBD-H** (right)



(z) **3a-CO2-TS** (left), **3b-CO2-TS** (right)

Table S17. Energies and Cartesian Coordinates of all structures

TBD_solv
E(TPSS-D3/def2-TZVP) = -439.0983684905 (conv)
Lowest Freq. = 72.81 cm^-1
23
TBD_solv (009/c1/tpss-d3.def2-TZVP_COSMO_37.5)

H	0.6261039	-1.3061880	2.4259964
C	1.0679743	-0.9303035	1.4956391
H	1.8704035	-0.2292001	1.7739315
N	0.0218587	-0.1945194	0.7720816
C	-0.7044124	0.7922934	1.5849032
H	-1.5531928	0.3018539	2.0819741
H	-0.0207256	1.1408000	2.3680733
C	-1.1836424	1.9576833	0.7296631
H	-1.8755989	2.5782354	1.3091897
H	-0.3280578	2.5800578	0.4399860
C	-1.8491918	1.4015173	-0.5291122
H	-2.7623737	0.8523068	-0.2425249
H	-2.1686418	2.2188664	-1.1861385
N	-0.9481738	0.5336940	-1.2869148
C	-0.1074795	-0.1870230	-0.5955209
N	0.6828674	-1.0909650	-1.2995560
C	1.9413498	-1.5754183	-0.7327282
H	2.7112609	-0.7873638	-0.6979939
H	2.3098233	-2.3815196	-1.3724187
C	1.6407195	-2.0768806	0.6733688
H	0.9199783	-2.8999910	0.6142704
H	2.5488250	-2.4477710	1.1579886
H	0.6967192	-0.8641172	-2.2883245

TBD_vac
E(TPSS-D3/def2-TZVP) = -439.0851453005 (conv)
Lowest Freq. = 68.91 cm^-1
23
TBD_vac (009/c1/tpss-d3.def2-TZVP)

H	0.6623801	-1.2995942	2.4402599
C	1.0747027	-0.9202151	1.4962071
H	1.8768548	-0.2079164	1.7585207

N 0.0059418 -0.2151092 0.7881817
C -0.7227510 0.7730739 1.5912312
H -1.5847595 0.2899091 2.0751450
H -0.0511635 1.1160862 2.3892985
C -1.1815480 1.9491169 0.7355003
H -1.8736402 2.5742269 1.3114739
H -0.3154687 2.5647097 0.4635672
C -1.8311467 1.4127666 -0.5423606
H -2.7631103 0.8813584 -0.2844841
H -2.1165752 2.2408446 -1.2011131
N -0.9370074 0.5341129 -1.2804976
C -0.1192815 -0.1921101 -0.5908206
N 0.6668800 -1.1073720 -1.2903602
C 1.9331465 -1.5699699 -0.7406894
H 2.7045573 -0.7791468 -0.7171333
H 2.3049957 -2.3808446 -1.3742997
C 1.6536672 -2.0653618 0.6736935
H 0.9382783 -2.8930877 0.6230710
H 2.5697908 -2.4266843 1.1524540
H 0.6416502 -0.8927455 -2.2810123

TBD-H_vac
E(TPSS-D3/def2-TZVP) = -439.5055842919 (conv)
Lowest Freq. = 73.79 cm^-1
24
TBD-H_vac (009-H/c1/tpss-d3.def2-TZVP)
H 0.7164184 -1.1568771 2.4239721
C 1.1681716 -0.8584683 1.4739726
H 2.0277684 -0.2137230 1.6948404
N 0.1526846 -0.0636997 0.7512086
C -0.7201376 0.7983710 1.5759470
H -1.5235184 0.1835555 2.0002818
H -0.1064740 1.1695292 2.4013757
C -1.2802426 1.9552789 0.7591223
H -2.0244543 2.4918277 1.3525824
H -0.4789487 2.6565243 0.5042748
C -1.9183974 1.4183910 -0.5155513
H -2.8134670 0.8258535 -0.2912439
H -2.2007374 2.2285410 -1.1908428
N -0.9270936 0.5858765 -1.2118065
C 0.0291317 -0.1215899 -0.5796251
N 0.8582593 -0.8890774 -1.3134005
C 1.9727640 -1.6580656 -0.7418997
H 2.8843908 -1.0483402 -0.7364317
H 2.1402131 -2.5238984 -1.3855188
C 1.5856807 -2.0820307 0.6690880
H 0.7615546 -2.8013785 0.6254817
H 2.4333297 -2.5666654 1.1596105
H 0.7605626 -0.8579522 -2.3192812
H -1.0136106 0.4699449 -2.2124452

TBD-CO2_solv
E(TPSS-D3/def2-TZVP) = -627.8245256622 (conv)
Lowest Freq. = 34.63 cm^-1
26
TBD-CO2_solv (009-CO2/c1/tpss-d3.def2-TZVP_COSMO_37.5)
H 0.7223108 0.0643265 2.7107716
C 1.0955926 0.6677279 1.8777642
H 1.3080138 1.6750509 2.2577247
N -0.0029933 0.7559461 0.8962857
C -1.3348656 0.9526472 1.4888150
H -1.6799348 -0.0032631 1.9024223
H -1.2155824 1.6574742 2.3182389
C -2.3043630 1.4777663 0.4485800
H -3.3249393 1.4230948 0.8365841
H -2.0813344 2.5240049 0.2120531
C -2.1779094 0.6308328 -0.8059488
H -2.4279107 -0.4164698 -0.5932407

H -2.8268053 0.9816602 -1.6044381
N -0.7996537 0.7127359 -1.3282505
C 0.2377968 0.7446319 -0.4294419
N 1.4917426 0.7480958 -0.8850819
C 2.6720602 0.7673293 -0.0262860
H 2.9754809 1.8024463 0.1762711
H 3.4803835 0.2745370 -0.5703879
C 2.3416013 0.0418847 1.2708434
H 2.1667586 -1.0194677 1.0647516
H 3.1693672 0.1240097 1.9797672
C -0.6365189 0.6704312 -2.7985866
O 0.5422444 0.7153976 -3.2537926
O -1.7021764 0.5918698 -3.4376000
H 1.5303971 0.7234421 -1.9202419

MTBD_solv
E(TPSS-D3/def2-TZVP) = -478.4267961429 (conv)
Lowest Freq. = 65.84 cm^-1
26
MTBD_solv (006/c1/tpss-d3.def2-TZVP_COSMO_37.5)
H 0.5654989 -1.3230545 2.4133089
C 1.0402661 -0.9449960 1.4993311
H 1.8516256 -0.2671992 1.8093927
N 0.0344997 -0.1793918 0.7567540
C -0.6636355 0.8218026 1.5775644
H -1.4865633 0.3344503 2.1198626
H 0.0497702 1.1888742 2.3262892
C -1.1905642 1.9682260 0.7276515
H -1.8834056 2.5759475 1.3196914
H -0.3603878 2.6100313 0.4080721
C -1.8679146 1.3758051 -0.5067937
H -2.7392293 0.7782000 -0.1867481
H -2.2534947 2.1710499 -1.1553632
N -0.9435808 0.5590408 -1.2895409
C -0.0872140 -0.1639857 -0.6189412
N 0.7329511 -1.0344153 -1.3326460
C 1.9501675 -1.5561324 -0.7119003
H 2.7349796 -0.7830026 -0.6427613
H 2.3276169 -2.3557434 -1.3553526
C 1.6044513 -2.0860494 0.6707391
H 0.8670938 -2.8905470 0.5729650
H 2.4930689 -2.4908320 1.1645191
C 0.7713084 -0.8773307 -2.7829660
H -0.2451271 -0.8187353 -3.1720957
H 1.2797267 -1.7504817 -3.2011688
H 1.3108722 0.0317393 -3.0907432

MTBD_vac
E(TPSS-D3/def2-TZVP) = -478.4166031370 (conv)
Lowest Freq. = 64.71 cm^-1
26
MTBD_vac (006/c1/tpss-d3.def2-TZVP)
H 0.5868635 -1.3239918 2.4210328
C 1.0480696 -0.9375103 1.5018449
H 1.8605725 -0.2569972 1.8126638
N 0.0349780 -0.1862499 0.7669934
C -0.6795174 0.8037079 1.5801780
H -1.5125334 0.3123034 2.1059536
H 0.0165825 1.1701142 2.3476059
C -1.1949909 1.9581860 0.7307230
H -1.8918614 2.5650313 1.3202230
H -0.3580436 2.5992570 0.4285828
C -1.8554184 1.3827222 -0.5226700
H -2.7443664 0.7972499 -0.2303013
H -2.2113379 2.1884220 -1.1746443
N -0.9319735 0.5587717 -1.2845235
C -0.0873717 -0.1616713 -0.6174547
N 0.7361580 -1.0358955 -1.3286823

C 1.9547500 -1.5424681 -0.7153785
H 2.7416525 -0.7675800 -0.6484337
H 2.3388267 -2.3415858 -1.3574738
C 1.6198344 -2.0745718 0.6704649
H 0.8853916 -2.8812628 0.5727255
H 2.5121003 -2.4759568 1.1623410
C 0.7543054 -0.8883275 -2.7790116
H -0.2660536 -0.7501446 -3.1334442
H 1.1872426 -1.7982571 -3.2068636
H 1.3489205 -0.0200253 -3.1033313

MTBD-H_vac
E(TPSS-D3/def2-TZVP) = -478.8393850453 (conv)
Lowest Freq. = 46.17 cm^-1
27
MTBD-H_vac (006-H/c1/tpss-d3.def2-TZVP)
H 0.6261362 -1.2174662 2.4141052
C 1.1226729 -0.8933288 1.4946526
H 1.9758885 -0.2631459 1.7756639
N 0.1527583 -0.0704206 0.7482161
C -0.6964390 0.8147964 1.5725987
H -1.5073544 0.2184602 2.0096594
H -0.0682482 1.1790073 2.3907472
C -1.2466079 1.9762811 0.7580455
H -1.9782564 2.5251080 1.3559286
H -0.4391715 2.6657296 0.4904754
C -1.8995745 1.4341116 -0.5057098
H -2.7925603 0.8441555 -0.2666774
H -2.1903355 2.2385142 -1.1841079
N -0.9194012 0.5965271 -1.2094721
C 0.0366650 -0.1252859 -0.5898860
N 0.8607603 -0.8883722 -1.3394453
C 1.9799344 -1.6188902 -0.7172011
H 2.8678591 -0.9745838 -0.6718916
H 2.2082007 -2.4680300 -1.3643325
C 1.5685490 -2.0888711 0.6696608
H 0.7538968 -2.8154040 0.5844131
H 2.4106818 -2.5804233 1.1631779
C 0.7620706 -0.8708908 -2.8030119
H -0.2356791 -1.1813059 -3.1335656
H 1.4815875 -1.5889300 -3.1939067
H 1.0041782 0.1169578 -3.2130625
H -0.9698127 0.5410924 -2.2156852

MTBD-CO2_solv
E(TPSS-D3/def2-TZVP) = -667.1426888662 (conv)
Lowest Freq. = 40.46 cm^-1
29
MTBD-CO2_solv (006-CO2/c1/tpss-d3.def2-TZVP_COSMO_37.5)
H 0.3806720 -1.2968821 2.2757516
C 1.0122334 -0.9297744 1.4598333
H 1.8312505 -0.3512661 1.9033366
N 0.1954171 0.0002181 0.6570491
C -0.5184160 0.9986031 1.4825500
H -1.1102820 0.4258084 2.2055724
H 0.2334670 1.5665107 2.0419067
C -1.4245389 1.9155071 0.6674620
H -2.2250981 2.2902249 1.3119408
H -0.8684531 2.7761986 0.2817471
C -1.9692723 1.1165670 -0.5111198
H -2.5073740 0.2243862 -0.1726393
H -2.6155871 1.7080132 -1.1563368
N -0.8237359 0.7006589 -1.3384234
C 0.1228609 -0.0454781 -0.6862687
N 0.9281938 -0.8620783 -1.3810704
C 2.0554607 -1.5154577 -0.7003754
H 2.8648318 -0.7912787 -0.5475567
H 2.4196124 -2.3024504 -1.3613513

C 1.5571936 -2.0767186 0.6244147
H 0.7763529 -2.8186912 0.4288369
H 2.3678781 -2.5665294 1.1699731
C 0.6920911 -1.1999809 -2.7841121
H -0.3277606 -0.9298674 -3.0561712
H 0.8269773 -2.2796736 -2.8973652
H 1.3904835 -0.6648561 -3.4321704
C -0.4177722 1.6408538 -2.4427311
O 0.7988940 1.6601723 -2.7171208
O -1.3712220 2.2843889 -2.9301046

DBN_solv
E(TPSS-D3/def2-TZVP) = -383.7107644686 (conv)
Lowest Freq. = 97.45 cm^-1
21
DBN_solv (008/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -4.4470289 -1.9232789 1.6418467
N -4.6436543 -0.4974159 1.4297876
C -3.0359419 -2.1239974 2.1989058
H -4.5789481 -2.4753267 0.6991756
H -5.2062246 -2.2801466 2.3466611
C -2.0121399 -1.3829548 1.3297629
H -2.9981595 -1.7310936 3.2220542
H -2.8009757 -3.1925828 2.2407167
C -3.5956429 0.3371600 1.1452037
N -2.3375666 0.0381058 1.0984020
H -1.9211991 -1.8875593 0.3557805
H -1.0231513 -1.4321392 1.7998344
C -4.1651171 1.7101776 0.8466498
C -5.6173175 1.6262432 1.3537773
H -4.1339874 1.8696465 -0.2386582
H -3.5777652 2.5020246 1.3171495
C -5.9515723 0.1282070 1.2453419
H -6.3083436 2.2474617 0.7799723
H -5.6648093 1.9331776 2.4033202
H -6.3737487 -0.1280398 0.2613215
H -6.6492063 -0.2141491 2.0167744

DBN_vac
E(TPSS-D3/def2-TZVP) = -383.7000610909 (conv)
Lowest Freq. = 92.85 cm^-1
21
DBN_vac (008/c1/tpss-d3.def2-TZVP)
C -4.4518264 -1.9188918 1.6451702
N -4.6530089 -0.4910757 1.4843062
C -3.0361852 -2.1315765 2.1905223
H -4.5830586 -2.4458599 0.6853956
H -5.2062617 -2.3075297 2.3402870
C -2.0111496 -1.3766782 1.3308346
H -2.9966192 -1.7530454 3.2187376
H -2.8037982 -3.2019759 2.2199490
C -3.5929929 0.3347186 1.1509063
N -2.3488225 0.0301473 1.0780324
H -1.8896364 -1.8842419 0.3618507
H -1.0298430 -1.4050557 1.8182154
C -4.1642935 1.7048802 0.8403896
C -5.6156798 1.6288771 1.3507475
H -4.1321794 1.8556358 -0.2458168
H -3.5715098 2.4977684 1.3005315
C -5.9510801 0.1289014 1.2604403
H -6.3099061 2.2453863 0.7746010
H -5.6626758 1.9462654 2.3973635
H -6.3609538 -0.1368353 0.2706559
H -6.6710192 -0.1962946 2.0206604

DBN-H_vac
E(TPSS-D3/def2-TZVP) = -384.1136388027 (conv)
Lowest Freq. = 109.75 cm^-1

22
DBN-H_vac (008-H/c1/tpss-d3.def2-TZVP)
C -4.4261616 -1.9299059 1.6219710
N -4.6383516 -0.4961381 1.3767422
C -3.0197948 -2.1348689 2.1906476
H -4.5703387 -2.4769055 0.6829158
H -5.1882838 -2.2638641 2.3302791
C -1.9679590 -1.4340423 1.3304869
H -2.9790375 -1.7417053 3.2114045
H -2.7981527 -3.2036109 2.2352687
C -3.6474201 0.3456211 1.1352513
N -2.3779135 -0.0311576 1.1127159
H -1.8519516 -1.9240849 0.3576053
H -0.9971780 -1.4241812 1.8296199
C -4.1612128 1.7278233 0.8529919
C -5.6274406 1.6446994 1.3352323
H -4.0905944 1.9091195 -0.2270815
H -3.5738375 2.4982567 1.3586391
C -5.9684282 0.1455693 1.2640156
H -6.2994276 2.2484403 0.7252008
H -5.6971530 1.9913885 2.3689898
H -6.4280399 -0.1456734 0.3127541
H -6.6070207 -0.1951122 2.0818497
H -1.6721862 0.6708772 0.9274219

DBN-CO2_solv
E(TPSS-D3/def2-TZVP) = -572.4272097305 (conv)
Lowest Freq. = 38.94 cm^-1
24
DBN-CO2_solv (008-CO2/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -0.3123634 -1.5736527 0.3004949
N -0.5041437 -0.1879115 -0.1393947
C 1.1248211 -1.7484411 0.7732177
H -0.5489276 -2.2427328 -0.5341729
H -1.0273833 -1.7652665 1.1055298
C 2.0833805 -1.1314197 -0.2388245
H 1.2578458 -1.2632013 1.7459453
H 1.3478200 -2.8118464 0.8894575
C 0.4793926 0.6687134 -0.4056666
N 1.7582343 0.2978616 -0.4409084
H 2.0214954 -1.6480495 -1.2033058
H 3.1156351 -1.1701299 0.1023761
C -0.0887958 2.0409322 -0.6564633
C -1.5915624 1.7634093 -0.8665203
H 0.3928285 2.5278122 -1.5018084
H 0.1053546 2.6601326 0.2255212
C -1.8390469 0.4401377 -0.1356242
H -1.7973429 1.6401286 -1.9331899
H -2.2194723 2.5683948 -0.4825108
H -2.5500159 -0.2161651 -0.6431811
H -2.1626308 0.5764979 0.9031461
C 2.9005981 1.2505386 -0.7258757
O 2.6152912 2.4597894 -0.6743374
O 3.9734447 0.6629466 -0.9615328

DBU_solv
E(TPSS-D3/def2-TZVP) = -462.3815185844 (conv)
Lowest Freq. = 63.79 cm^-1
27
DBU_solv (007/c2/tpss-d3.def2-TZVP_COSMO_37.5)
H -0.2175680 -2.5943542 1.2579085
C 0.4257490 -1.7137885 1.3723470
H 0.3652524 -1.4119046 2.4217352
N -0.1277268 -0.5960911 0.5977847
C -0.1314385 0.7110542 1.2740081
H -0.9746755 0.7561317 1.9771947
H 0.7921089 0.7903208 1.8595444
C -0.2200410 1.8381695 0.2545798

H -0.4352431 2.7819761 0.7662425
H 0.7399078 1.9457398 -0.2649301
C -1.3038665 1.4926552 -0.7674922
H -2.2808296 1.4377758 -0.2608363
H -1.3838756 2.2768262 -1.5285700
N -1.0251085 0.2219406 -1.4461188
C -0.4717612 -0.7097452 -0.7234213
C 1.8753260 -2.0696456 1.0109535
C -0.1490524 -2.0198075 -1.4061320
C 1.3661433 -2.3033024 -1.5151052
H -0.5870585 -1.9501856 -2.4043911
H -0.6407162 -2.8556394 -0.8898788
C 1.9867678 -2.9242800 -0.2568074
H 2.3145267 -2.6231634 1.8505190
H 2.4501859 -1.1403167 0.9025115
H 1.8855606 -1.3708466 -1.7736303
H 1.5228800 -2.9942474 -2.3518253
H 1.4924541 -3.8882609 -0.0672920
H 3.0435115 -3.1460968 -0.4508777

DBU_vac
E(TPSS-D3/def2-TZVP) = -462.3710307178 (conv)
Lowest Freq. = 60.55 cm^-1
27
DBU_vac (007/c2/tpss-d3.def2-TZVP)
H -0.2099358 -2.5896911 1.2723005
C 0.4355686 -1.7081724 1.3775130
H 0.3849866 -1.4086955 2.4293421
N -0.1179347 -0.5937644 0.6086329
C -0.1399285 0.7105689 1.2803269
H -0.9916457 0.7557864 1.9760880
H 0.7760287 0.8041266 1.8786767
C -0.2269215 1.8368613 0.2573107
H -0.4430577 2.7825690 0.7668245
H 0.7363349 1.9437777 -0.2559509
C -1.3010015 1.4879151 -0.7761041
H -2.2864616 1.4420100 -0.2850058
H -1.3665018 2.2664565 -1.5439610
N -1.0239040 0.2166889 -1.4400776
C -0.4725355 -0.7060845 -0.7219370
C 1.8824512 -2.0751685 1.0092386
C -0.1509625 -2.0157474 -1.4061039
C 1.3621173 -2.3032529 -1.5164846
H -0.5901675 -1.9314924 -2.4017180
H -0.6470415 -2.8543952 -0.8968211
C 1.9846264 -2.9276929 -0.2608791
H 2.3261432 -2.6318229 1.8452770
H 2.4615533 -1.1487736 0.8983373
H 1.8812064 -1.3712525 -1.7754025
H 1.5203794 -2.9925496 -2.3545534
H 1.4883343 -3.8908252 -0.0699668
H 3.0396824 -3.1564651 -0.4568817

DBU-H_vac
E(TPSS-D3/def2-TZVP) = -462.7891760592 (conv)
Lowest Freq. = 75.31 cm^-1
28
DBU-H_vac (007-H/c2/tpss-d3.def2-TZVP)
H -0.1650994 -2.5685845 1.3215099
C 0.5035014 -1.7037200 1.3896840
H 0.4837837 -1.3616333 2.4259507
N -0.0803792 -0.5894351 0.5988011
C -0.2389476 0.7108099 1.2924090
H -1.1568268 0.6744439 1.8906569
H 0.6071505 0.8112751 1.9764833
C -0.2634723 1.8640401 0.2961378
H -0.5232873 2.7882340 0.8174325
H 0.7296948 1.9941116 -0.1458537

C -1.2798238 1.5810573 -0.8041648
H -2.3055913 1.6045033 -0.4195109
H -1.2011238 2.3030600 -1.6193181
N -0.9982557 0.2470649 -1.3551472
C -0.4282940 -0.7450681 -0.6699817
C 1.9287222 -2.0724841 0.9649563
C -0.1604701 -2.0338612 -1.3919259
C 1.3502341 -2.3393446 -1.5431630
H -0.6307767 -1.9698903 -2.3774053
H -0.6565498 -2.8540491 -0.8584537
C 1.9883883 -2.9502483 -0.2904677
H 2.3885291 -2.6161408 1.7974049
H 2.5115551 -1.1527984 0.8287620
H 1.8758355 -1.4236593 -1.8408928
H 1.4550125 -3.0455610 -2.3723181
H 1.4910978 -3.9056432 -0.0747548
H 3.0341618 -3.1883060 -0.5095416
H -1.2326541 0.0588040 -2.3214044

DBU-CO2_solv
E(TPSS-D3/def2-TZVP) = -651.0920556383 (conv)
Lowest Freq. = 28.88 cm^-1
30
DBU-CO2_solv (007-CO2/c1/tpss-d3.def2-TZVP_COSMO_37.5)
H 1.6392724 -0.2639551 2.1169150
C 1.6281790 -0.6233340 1.0875193
H 2.5215371 -0.2252928 0.5931553
N 0.4193475 -0.0208197 0.4801021
C -0.4944581 0.6940393 1.3917715
H -1.2036748 -0.0193649 1.8280445
H 0.1147016 1.1082831 2.1970554
C -1.2142922 1.7887854 0.6233031
H -1.9509411 2.2743669 1.2682971
H -0.4908283 2.5440102 0.2980919
C -1.9103717 1.1778147 -0.5781342
H -2.7563577 0.5543803 -0.2653371
H -2.2797802 1.9370870 -1.2674593
N -0.9753620 0.3382006 -1.3558684
C 0.1450257 -0.1531676 -0.8223156
C 1.6324980 -2.1577079 1.0721633
C 1.1666987 -0.8404090 -1.6862748
C 1.2313974 -2.3687756 -1.4643715
H 2.1424706 -0.3948059 -1.4563674
H 0.9399947 -0.6264194 -2.7268003
C 2.0876619 -2.7667601 -0.2585929
H 0.6314476 -2.5164195 1.3425739
H 2.3157893 -2.4874296 1.8634147
H 1.6582599 -2.8161803 -2.3679399
H 0.2124132 -2.7579415 -1.3681123
H 2.0994490 -3.8592575 -0.1683088
H 3.1242600 -2.4530808 -0.4459755
C -1.4368830 0.0297877 -2.7888067
O -2.0068441 0.9921998 -3.3318344
O -1.2202963 -1.1316868 -3.1719639

2a_solv
E(TPSS-D3/def2-TZVP) = -710.8449308134 (conv)
Lowest Freq. = 14.89 cm^-1
38
2a_solv (012/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -0.2533216 -0.9915527 -0.4411693
C 1.1028782 -0.5971702 -0.3910335
N -1.0179392 0.0751450 0.0419747
N 1.1359244 0.6924129 0.1136498
C -0.1692535 1.1512579 0.3657191
N -0.3767263 2.3532816 0.7796940
C -2.4325348 -0.0410505 0.4644699
C -3.3694460 -0.1592997 -0.7417860

H -2.6545298 0.8922867 0.9741189
C -2.6171409 -1.1676771 1.4888263
C 2.3107828 1.5650949 0.2682845
C 2.9724583 1.8542913 -1.0836942
C 3.2836122 1.0045949 1.3110851
H 1.8812422 2.4938543 0.6520926
C -1.6904613 2.9746362 0.8569977
H -1.5466596 4.0603273 0.8784039
H -2.2381545 2.7097122 1.7742488
H -2.3357069 2.7452358 -0.0038961
C 2.1152970 -1.4571123 -0.8133958
C -0.6143178 -2.2484045 -0.9174143
C 1.7466940 -2.7237751 -1.2895144
H 3.1587512 -1.1675249 -0.7803036
C 0.4067112 -3.1134227 -1.3407997
H -1.6493530 -2.5631641 -0.9711751
H 2.5212343 -3.4072896 -1.6251338
H 0.1429014 -4.0981554 -1.7151027
H -2.4394174 -2.1550693 1.0558375
H -3.6449065 -1.1406550 1.8641166
H -1.9352779 -1.0299899 2.3336281
H 3.7316542 0.0604305 0.9866841
H 2.7692036 0.8351036 2.2619992
H 4.0926338 1.7232576 1.4764858
H -3.2013517 -1.0850226 -1.2988226
H -3.2248503 0.6848264 -1.4231390
H -4.4081788 -0.1544738 -0.3968496
H 2.2442690 2.2774438 -1.7826125
H 3.3982938 0.9513232 -1.5312503
H 3.7818064 2.5782133 -0.9449341

2a_vac
E(TPSS-D3/def2-TZVP) = -710.8349694309 (conv)
Lowest Freq. = 19.35 cm^-1
38
2a_vac (012/c1/tpss-d3.def2-TZVP)
C -0.2515670 -1.0076300 -0.4356694
C 1.1021093 -0.6047961 -0.4009716
N -1.0176747 0.0614738 0.0431057
N 1.1326225 0.6884385 0.0927010
C -0.1715352 1.1462769 0.3607760
N -0.3658557 2.3424347 0.7800610
C -2.4352246 -0.0384276 0.4354889
C -3.3478186 -0.1837168 -0.7881569
H -2.6654080 0.9108772 0.9126055
C -2.6488752 -1.1384613 1.4841961
C 2.2970613 1.5691930 0.2505753
C 2.9591168 1.8651118 -1.0998818
C 3.2712607 1.0177729 1.2971773
H 1.8527365 2.4924405 0.6336959
C -1.6554584 2.9805308 0.9346424
H -1.4882559 4.0597754 1.0143639
H -2.1810456 2.6746289 1.8539972
H -2.3359078 2.8177877 0.0833403
C 2.1136907 -1.4637450 -0.8235258
C -0.6069208 -2.2709946 -0.8951474
C 1.7497883 -2.7363332 -1.2828617
H 3.1552018 -1.1663297 -0.8010260
C 0.4141937 -3.1341849 -1.3183354
H -1.6405196 -2.5928291 -0.9364252
H 2.5249889 -3.4189788 -1.6175747
H 0.1536996 -4.1240892 -1.6799915
H -2.4337172 -2.1335301 1.0876321
H -3.6906419 -1.1227848 1.8207615
H -2.0019690 -0.9681560 2.3498491
H 3.7194603 0.0701078 0.9830838
H 2.7554487 0.8549835 2.2479606
H 4.0807595 1.7366885 1.4610652

H -3.1671119 -1.1196322 -1.3230333
H -3.1852152 0.6438592 -1.4849611
H -4.3957279 -0.1709353 -0.4709260
H 2.2298422 2.2925209 -1.7942810
H 3.3812845 0.9646507 -1.5560674
H 3.7700050 2.5879218 -0.9619527

2a-H_vac
E(TPSS-D3/def2-TZVP) = -711.2484489152 (conv)
Lowest Freq. = 46.52 cm^-1
39
2a-H_vac (012-H/c1/tpss-d3.def2-TZVP)
C -0.2455445 -1.0014605 -0.4407991
C 1.1007593 -0.6034900 -0.3841100
N -1.0068897 0.0372834 0.1264747
N 1.1201458 0.6894195 0.1698347
C -0.1592022 1.0408124 0.4704949
N -0.5271955 2.2026899 1.0568098
C -2.4292162 -0.0643014 0.5733742
C -3.3788263 -0.1048752 -0.6247815
H -2.6040475 0.8527312 1.1373349
C -2.6021451 -1.2416652 1.5374283
C 2.3071972 1.5799909 0.2911008
C 2.9378691 1.8363102 -1.0807989
C 3.2859646 1.0366221 1.3351124
H 1.9095062 2.5342589 0.6500326
C -1.6620805 3.0369338 0.6098663
H -1.2951440 4.0402947 0.3802927
H -2.4288302 3.1036924 1.3856489
H -2.0918801 2.6115250 -0.2974490
C 2.1227213 -1.4334076 -0.8414754
C -0.6153443 -2.2337738 -0.9757752
C 1.7509662 -2.6677303 -1.3695155
H 3.1649533 -1.1450352 -0.7965624
C 0.4069011 -3.0597630 -1.4375523
H -1.6489790 -2.5492059 -1.0358804
H 2.5210726 -3.3369581 -1.7379786
H 0.1541872 -4.0273768 -1.8576945
H -2.4552784 -2.2041452 1.0435646
H -3.6193802 -1.2184902 1.9378928
H -1.9011354 -1.1675946 2.3733585
H 3.7169250 0.0825919 1.0222406
H 2.7927091 0.8914884 2.3004094
H 4.1037198 1.7501717 1.4670012
H -3.2434799 -1.0128777 -1.2171345
H -3.2285304 0.7563441 -1.2823454
H -4.4110606 -0.0881812 -0.2649509
H 2.1959912 2.2193976 -1.7868579
H 3.3831386 0.9327893 -1.5013622
H 3.7288236 2.5830170 -0.9705262
H 0.2203533 2.7029900 1.5185825

2a-CO2_solv
E(TPSS-D3/def2-TZVP) = -899.5582318895 (conv)
Lowest Freq. = 33.13 cm^-1
41
2a-CO2_solv (012-CO2/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -0.2134266 -1.0381793 -0.3598443
C 1.1301285 -0.6110002 -0.4129841
N -0.9436925 0.0084646 0.2045394
N 1.1604745 0.6875305 0.0936801
C -0.0964602 1.0389391 0.4666102
N -0.4563034 2.2451421 0.9902030
C -2.3739014 -0.0018708 0.6106488
C -3.2871234 -0.0959394 -0.6123856
H -2.5183251 0.9671195 1.0910713
C -2.6218501 -1.0952190 1.6524738
C 2.3292227 1.6019166 0.1714320

C 2.8521930 1.9134110 -1.2328071
C 3.3906989 1.0428621 1.1191488
H 1.9169261 2.5141343 0.6056287
C -1.3771742 3.1299551 0.2576109
H -0.9365234 4.1279329 0.2026626
H -2.3481254 3.1989132 0.7571479
H -1.5116941 2.7418144 -0.7542294
C 2.1338233 -1.4385225 -0.9214648
C -0.5932064 -2.3015425 -0.8168056
C 1.7505297 -2.6980251 -1.3739480
H 3.1686486 -1.1243463 -0.9704107
C 0.4114340 -3.1226992 -1.3215305
H -1.6210134 -2.6404053 -0.7847340
H 2.5052988 -3.3652063 -1.7778960
H 0.1518751 -4.1127128 -1.6826755
H -2.4998214 -2.0962388 1.2311023
H -3.6482593 -1.0017229 2.0180936
H -1.9380591 -0.9817359 2.4983275
H 3.8483633 0.1310444 0.7256156
H 2.9458188 0.8353164 2.0945719
H 4.1787194 1.7917295 1.2415877
H -3.1814798 -1.0569921 -1.1225756
H -3.0687681 0.7041471 -1.3252198
H -4.3256558 0.0036348 -0.2848286
H 2.0530428 2.3113398 -1.8650915
H 3.2751421 1.0289633 -1.7166153
H 3.6405276 2.6673068 -1.1527999
C -0.0256265 2.5853084 2.3511506
O 0.6568875 1.6996632 2.9204425
O -0.4093315 3.7061629 2.7516742

2b_solv
E(TPSS-D3/def2-TZVP) = -828.8533057687 (conv)
Lowest Freq. = 7.37 cm^-1
47
2b_solv (013/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -0.2008560 -1.1854966 -0.3401590
C 1.1156282 -0.6733026 -0.4088567
N -1.0305558 -0.1491285 0.0890063
N 1.0579368 0.6506539 -0.0246309
C -0.2716889 1.0286278 0.2988547
N -0.4956360 2.2280830 0.6748796
C -2.4854194 -0.2721388 0.2649704
C -3.1919222 -0.5668706 -1.0635369
H -2.8055680 0.7119779 0.5927219
C -2.8390588 -1.2659454 1.3776527
C 2.1698368 1.6056736 0.0692718
C 2.7970394 1.8686301 -1.3041505
C 3.1887459 1.1741214 1.1296660
H 1.6729380 2.5183443 0.4097103
C -1.6566216 3.0007222 1.1006831
C -1.0875493 4.4000423 1.4291262
C -2.2977902 2.4611540 2.3979446
C -2.6964466 3.1923439 -0.0251598
C 2.1786625 -1.4817717 -0.8100244
C -0.4676254 -2.5109397 -0.6727290
C 1.9041834 -2.8167238 -1.1432574
H 3.1913705 -1.1007505 -0.8665420
C 0.6049584 -3.3229296 -1.0764150
H -1.4686687 -2.9216728 -0.6273755
H 2.7201707 -3.4612676 -1.4574802
H 0.4124712 -4.3590986 -1.3389277
H -2.5576414 -2.2898321 1.1193911
H -3.9195272 -1.2439415 1.5513252
H -2.3314227 -0.9930971 2.3080177
H 3.6958544 0.2430716 0.8580467
H 2.6942582 1.0299734 2.0954028
H 3.9499666 1.9531070 1.2424600

H -2.9252477 -1.5490384 -1.4618471
H -2.9314346 0.1903316 -1.8095577
H -4.2752892 -0.5451209 -0.9090560
H 2.0331318 2.2031581 -2.0130317
H 3.2811680 0.9761891 -1.7127013
H 3.5551269 2.6536379 -1.2148582
H -2.1965067 3.5825307 -0.9179296
H -3.4574447 3.9154363 0.2899023
H -3.2086824 2.2678216 -0.3016432
H -2.7868758 1.4931553 2.2675689
H -3.0497880 3.1695750 2.7637888
H -1.5248952 2.3497262 3.1657959
H -0.6092758 4.8232141 0.5398760
H -0.3338581 4.3172717 2.2189241
H -1.8814314 5.0777531 1.7636526

2b_vac
E(TPSS-D3/def2-TZVP) = -828.8463081664 (conv)
Lowest Freq. = 12.74 cm^-1
47
2b_vac (013/c1/tpss-d3.def2-TZVP)
C -0.2000883 -1.1887727 -0.3410702
C 1.1138971 -0.6763306 -0.4086256
N -1.0306709 -0.1504090 0.0892723
N 1.0550817 0.6489844 -0.0224266
C -0.2722515 1.0268051 0.2998290
N -0.4970869 2.2267204 0.6760799
C -2.4813071 -0.2724659 0.2654642
C -3.1886749 -0.5650638 -1.0639364
H -2.8015488 0.7116649 0.5947230
C -2.8341426 -1.2675332 1.3782538
C 2.1643365 1.6041946 0.0714115
C 2.7900353 1.8682250 -1.3026957
C 3.1830860 1.1733141 1.1325162
H 1.6673794 2.5171430 0.4121057
C -1.6550901 3.0014608 1.1002183
C -1.0837061 4.4004653 1.4264726
C -2.2977561 2.4655856 2.3986599
C -2.6956254 3.1938138 -0.0252885
C 2.1757722 -1.4836187 -0.8104593
C -0.4655497 -2.5129145 -0.6748577
C 1.9025792 -2.8161664 -1.1450551
H 3.1878546 -1.1012775 -0.8661353
C 0.6056067 -3.3228585 -1.0790869
H -1.4665271 -2.9240703 -0.6297475
H 2.7180964 -3.4600673 -1.4602216
H 0.4146837 -4.3584798 -1.3429559
H -2.5328033 -2.2875067 1.1285089
H -3.9162674 -1.2629377 1.5454361
H -2.3373262 -0.9848027 2.3110554
H 3.6819613 0.2358282 0.8688625
H 2.6890183 1.0384823 2.0992444
H 3.9507531 1.9466758 1.2412652
H -2.9039496 -1.5361863 -1.4757045
H -2.9406501 0.2035167 -1.8019421
H -4.2729660 -0.5636023 -0.9114306
H 2.0262332 2.2107388 -2.0070791
H 3.2636507 0.9739469 -1.7188366
H 3.5545909 2.6473278 -1.2156226
H -2.1948582 3.5762357 -0.9203745
H -3.4529573 3.9229097 0.2847198
H -3.2136078 2.2712056 -0.2985225
H -2.7877857 1.4973233 2.2714244
H -3.0485449 3.1746245 2.7657522
H -1.5254360 2.3535808 3.1663538
H -0.6047378 4.8218855 0.5374220
H -0.3292465 4.3181757 2.2148235
H -1.8747342 5.0814892 1.7609700

2b-H_vac
E(TPSS-D3/def2-TZVP) = -829.2681843556 (conv)
Lowest Freq. = 17.68 cm^-1
48
2b-H_vac (013-H/c1/tpss-d3.def2-TZVP)
C -0.2216813 -1.2031639 -0.1527394
C 1.0617464 -0.6345824 -0.2604922
N -1.1303364 -0.1432911 -0.0395762
N 0.8946365 0.7538718 -0.1795513
C -0.4349649 1.0252175 -0.0576814
N -1.0038190 2.2640811 -0.0496025
C -2.6122628 -0.2235125 -0.1988974
C -2.9541771 -0.6650100 -1.6245748
H -2.9400129 0.8087738 -0.0643569
C -3.2595019 -1.1030675 0.8732260
C 1.9731387 1.7782626 -0.1501838
C 2.7177945 1.8232848 -1.4866808
C 2.8842758 1.5690239 1.0622217
H 1.4440117 2.7247747 -0.0123220
C -1.5684310 2.9529350 1.1907714
C -0.5951651 4.0806332 1.5638620
C -1.6790817 1.9597036 2.3461220
C -2.9373018 3.5317717 0.8197322
C 2.1992164 -1.4291632 -0.4104852
C -0.4054400 -2.5861158 -0.1949518
C 2.0106214 -2.8067915 -0.4475349
H 3.1915895 -1.0054612 -0.4952702
C 0.7306724 -3.3745072 -0.3452736
H -1.3852128 -3.0387171 -0.1219482
H 2.8731758 -3.4550344 -0.5596974
H 0.6226013 -4.4532031 -0.3852333
H -3.0938157 -2.1659579 0.6851768
H -4.3392078 -0.9311040 0.8599362
H -2.8853960 -0.8691197 1.8729669
H 3.4527875 0.6393999 0.9906921
H 2.3040612 1.5494218 1.9890686
H 3.5959268 2.3972325 1.1172203
H -2.5912625 -1.6758482 -1.8290937
H -2.5216588 0.0190909 -2.3597694
H -4.0407658 -0.6623764 -1.7478815
H 2.0257616 1.9824358 -2.3186930
H 3.2729800 0.9011128 -1.6729197
H 3.4328283 2.6501887 -1.4691254
H -2.8543782 4.2131230 -0.0324835
H -3.3503418 4.0902933 1.6649786
H -3.6428048 2.7378681 0.5569505
H -2.4114755 1.1759707 2.1439756
H -2.0101641 2.4971778 3.2383976
H -0.7135693 1.4945357 2.5722519
H -0.4477143 4.7671383 0.7216259
H 0.3764858 3.6802334 1.8710573
H -0.9997979 4.6629425 2.3966634
H -0.4896386 2.9271149 -0.6216036

2b-CO2_solv
E(TPSS-D3/def2-TZVP) = -1017.572849816 (conv)
Lowest Freq. = 28.33 cm^-1
50
2b-CO2_solv (013-CO2/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -0.2533642 -1.1519230 -0.2691853
C 1.0481402 -0.6249206 -0.1289390
N -1.1289510 -0.0685067 -0.2410764
N 0.9106499 0.7574155 -0.0213083
C -0.4081073 1.0754591 -0.1038752
N -0.9279025 2.3449870 -0.0501948
C -2.5938054 -0.0844380 -0.4863411
C -2.8822922 -0.5720924 -1.9079544

H -2.8749796 0.9679761 -0.4151203
C -3.3304438 -0.8743397 0.5960199
C 1.9937809 1.7733223 0.0096090
C 2.7938354 1.7272440 -1.2941717
C 2.8549386 1.6298370 1.2649324
H 1.4528847 2.7204887 0.0532596
C -1.3301878 2.9843559 1.2616416
C -0.5027954 4.2598273 1.4821448
C -1.0530771 1.9985717 2.4030947
C -2.8304511 3.3132457 1.2301609
C 2.1707417 -1.4564548 -0.1183196
C -0.4697600 -2.5256185 -0.4027865
C 1.9492703 -2.8236724 -0.2523457
H 3.1750660 -1.0660582 -0.0137701
C 0.6519970 -3.3489398 -0.3920817
H -1.4622312 -2.9434720 -0.5131353
H 2.7992407 -3.4985809 -0.2492878
H 0.5203279 -4.4213939 -0.4945529
H -3.0968827 -1.9412122 0.5536894
H -4.4066710 -0.7566287 0.4413866
H -3.0825053 -0.5033752 1.5942760
H 3.4330166 0.7022415 1.2604258
H 2.2416958 1.6529669 2.1699554
H 3.5577022 2.4669020 1.3024447
H -2.6176275 -1.6254697 -2.0364704
H -2.3256311 0.0290684 -2.6312790
H -3.9525338 -0.4628021 -2.1053613
H 2.1224349 1.8302640 -2.1504131
H 3.3587714 0.7958232 -1.3901254
H 3.5040115 2.5590962 -1.2989714
H -3.0584898 3.9615815 0.3824291
H -3.1098052 3.8238722 2.1579686
H -3.4272956 2.3982187 1.1539332
H -1.6311422 1.0759453 2.2949369
H -1.3462468 2.4692437 3.3458375
H 0.0081548 1.7417968 2.4721177
H -0.6369932 4.9473918 0.6453433
H 0.5608355 4.0199656 1.5836367
H -0.8295734 4.7497593 2.4055834
C -1.0431806 2.9787643 -1.3638731
O -1.5081064 4.1371376 -1.4063684
O -0.6413543 2.2375449 -2.3020100

2c_solv
E(TPSS-D3/def2-TZVP) = -671.5263770734 (conv)
Lowest Freq. = 35.70 cm^-1
35
2c_solv (014/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -0.1770339 -1.1627887 -0.3956928
C 1.1535089 -0.6833870 -0.4278651
N -0.9714450 -0.1326050 0.0942531
N 1.1271174 0.6280985 0.0450797
C -0.1854841 0.9834686 0.3732461
N -0.6675182 2.0911887 0.8435055
C -2.4279296 -0.1375076 0.3162401
C -3.1882651 -0.3130365 -1.0025368
H -2.6284485 0.8639463 0.7049837
C -2.8218906 -1.1653284 1.3822434
C 2.2757001 1.5366697 0.1951496
C 2.9131663 1.8568582 -1.1613371
C 3.2758632 1.0034743 1.2268546
H 1.8514085 2.4638053 0.5908279
C 2.1947765 -1.4910384 -0.8758474
C -0.4825173 -2.4560269 -0.8114018
C 1.8833426 -2.7937191 -1.2939303
H 3.2187428 -1.1384785 -0.9063575
C 0.5696050 -3.2668924 -1.2622674
H -1.4969994 -2.8358070 -0.7921060

H 2.6820546 -3.4393238 -1.6469148
H 0.3521594 -4.2788949 -1.5908975
H -2.6259774 -2.1896457 1.0513356
H -3.8920968 -1.0764737 1.5937642
H -2.2680606 -0.9878781 2.3091316
H 3.7465879 0.0753725 0.8908210
H 2.7763909 0.8146645 2.1817217
H 4.0634340 1.7464500 1.3854130
H -3.0096996 -1.2967773 -1.4468507
H -2.8876054 0.4533875 -1.7233362
H -4.2626019 -0.2146778 -0.8177139
H 2.1639905 2.2559734 -1.8515554
H 3.3660319 0.9704281 -1.6138472
H 3.6973559 2.6077622 -1.0247661
H 0.0711871 2.7821690 0.9780232

2c_vac
E(TPSS-D3/def2-TZVP) = -671.5129567008 (conv)
Lowest Freq. = 37.36 cm^-1
35
2c_vac (014/c1/tpss-d3.def2-TZVP)
C -0.1724915 -1.1685080 -0.3972453
C 1.1580410 -0.6894909 -0.4288748
N -0.9676157 -0.1402980 0.0921295
N 1.1305530 0.6230921 0.0447040
C -0.1869504 0.9830692 0.3748423
N -0.6865876 2.0749308 0.8424061
C -2.4203886 -0.1341061 0.3160488
C -3.1841934 -0.3040880 -1.0016702
H -2.6066118 0.8714014 0.7039754
C -2.8203384 -1.1571967 1.3846753
C 2.2708462 1.5309040 0.1941784
C 2.9083840 1.8580624 -1.1618378
C 3.2755596 1.0040216 1.2263703
H 1.8396650 2.4557190 0.5915039
C 2.1971928 -1.4974167 -0.8766898
C -0.4746689 -2.4610068 -0.8139830
C 1.8877388 -2.7997397 -1.2953630
H 3.2212186 -1.1442163 -0.9070101
C 0.5764398 -3.2717337 -1.2643758
H -1.4897750 -2.8392344 -0.7952349
H 2.6862942 -3.4452159 -1.6478200
H 0.3595674 -4.2833725 -1.5934521
H -2.6197912 -2.1838940 1.0634954
H -3.8915402 -1.0706260 1.5938276
H -2.2708387 -0.9731262 2.3122961
H 3.7365588 0.0686019 0.8979324
H 2.7787823 0.8231269 2.1837899
H 4.0708769 1.7406809 1.3788969
H -3.0022487 -1.2826510 -1.4563669
H -2.8863695 0.4684655 -1.7163677
H -4.2595055 -0.2100968 -0.8183333
H 2.1598013 2.2675435 -1.8460939
H 3.3455687 0.9694437 -1.6248639
H 3.7028958 2.5993861 -1.0289663
H 0.0227812 2.7909986 0.9908465

2c-H_vac
E(TPSS-D3/def2-TZVP) = -671.9200156748 (conv)
Lowest Freq. = 44.39 cm^-1
36
2c-H_vac (014-H/c1/tpss-d3.def2-TZVP)
C -0.1793073 -1.1635071 -0.4019309
C 1.1413796 -0.6872757 -0.4380955
N -0.9797647 -0.1140585 0.0928625
N 1.1116552 0.6390655 0.0380248
C -0.1721860 0.9438883 0.3409266
N -0.5795531 2.1165932 0.8757405

C -2.4509921 -0.1554827 0.3271900
C -3.2033542 -0.3402130 -0.9931084
H -2.7097421 0.8287407 0.7293850
C -2.7958959 -1.1957608 1.3962863
C 2.2817333 1.5452899 0.2151384
C 2.9214775 1.8723873 -1.1364574
C 3.2557019 0.9694483 1.2466447
H 1.8721748 2.4709277 0.6305865
C 2.1886998 -1.4869085 -0.8890944
C -0.4961894 -2.4554868 -0.8142356
C 1.8703038 -2.7799790 -1.3003420
H 3.2112519 -1.1341844 -0.9250108
C 0.5531903 -3.2552214 -1.2633960
H -1.5087832 -2.8367883 -0.7933686
H 2.6625740 -3.4294428 -1.6567867
H 0.3411447 -4.2670457 -1.5917140
H -2.5730468 -2.2102419 1.0591211
H -3.8654470 -1.1387745 1.6152663
H -2.2419077 -1.0065332 2.3196501
H 3.7163961 0.0439625 0.8948717
H 2.7480306 0.7675030 2.1936298
H 4.0516996 1.6965824 1.4276921
H -2.9991815 -1.3150251 -1.4409708
H -2.9296774 0.4356544 -1.7135201
H -4.2779079 -0.2737540 -0.8030865
H 2.1865125 2.2930292 -1.8284581
H 3.3631824 0.9868607 -1.5982505
H 3.7165284 2.6075748 -0.9859939
H 0.0328572 2.9174484 0.8107438
H -1.5670739 2.3294182 0.8795236

2c-CO2_solv
E(TPSS-D3/def2-TZVP) = -860.2303683620 (conv)
Lowest Freq. = 39.66 cm^-1
38
2c-CO2_solv (014-CO2/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -0.1956133 -1.2308150 -0.3182735
C 1.1071628 -0.7051601 -0.4241428
N -1.0332980 -0.1749984 0.0551001
N 1.0237898 0.6474794 -0.0795900
C -0.2775689 0.9427687 0.1923208
N -0.7527403 2.1696245 0.5152448
C -2.5224967 -0.1879726 0.0809546
C -3.0658929 -0.4904766 -1.3178963
H -2.7913924 0.8314490 0.3549854
C -3.0424896 -1.1336677 1.1629506
C 2.1517486 1.6020353 0.0801893
C 2.8050482 1.8978237 -1.2709992
C 3.1305914 1.1031602 1.1461374
H 1.6880784 2.5170683 0.4546411
C 2.1842724 -1.5032380 -0.8099012
C -0.4576945 -2.5741613 -0.5894638
C 1.9183551 -2.8447679 -1.0787088
H 3.1890681 -1.1106103 -0.9005614
C 0.6207610 -3.3700542 -0.9715787
H -1.4532684 -2.9924693 -0.5156952
H 2.7347540 -3.4943083 -1.3779482
H 0.4492761 -4.4187063 -1.1927890
H -2.8208260 -2.1795309 0.9342274
H -4.1293483 -1.0257788 1.2266440
H -2.6059822 -0.8715124 2.1283765
H 3.6535057 0.1975988 0.8295545
H 2.6072521 0.8987979 2.0843939
H 3.8764837 1.8825172 1.3252144
H -2.8191566 -1.5049230 -1.6423978
H -2.6689053 0.2193663 -2.0495739
H -4.1554281 -0.3952653 -1.2970135
H 2.0640639 2.2622629 -1.9881006

H 3.2887868 1.0100764 -1.6870870
H 3.5675142 2.6696349 -1.1336807
H -0.2448858 2.9582866 0.1289963
C -1.4243696 2.4891306 1.8187521
O -1.7428704 1.5042356 2.5098358
O -1.5560470 3.7166121 1.9963492

2x_vac
E(TPSS-D3/def2-TZVP) = -553.4805610582 (conv)
Lowest Freq. = 33.78 cm^-1
26
2x_vac (003/c1/tpss-d3.def2-TZVP)
C -0.7128168 -0.7138719 -0.0101289
C 0.6880496 -0.8679813 0.0006726
N -0.9795446 0.6537844 0.0274792
N 1.2346929 0.4000414 0.0314415
C 0.2283723 1.3841066 0.0254264
N 0.5278977 2.6286847 0.0135590
C -2.3361636 1.1734706 0.0721787
H -2.8031912 1.1580913 -0.9203428
H -2.3331859 2.1906035 0.4528540
H -2.9285759 0.5494480 0.7491184
C 2.6473491 0.7205414 0.0211392
H 3.1251573 0.3211679 -0.8809195
H 3.1416774 0.3022533 0.9052637
H 2.7240184 1.8086458 0.0315272
C -0.4425384 3.7030379 -0.0500117
H 0.0971141 4.6332422 -0.2522748
H -0.9803036 3.8472442 0.9007356
H -1.1899704 3.5783130 -0.8488404
C 1.2735328 -2.1276865 -0.0192495
C -1.5597824 -1.8121103 -0.0458332
C 0.4173103 -3.2397953 -0.0520422
H 2.3519713 -2.2495453 -0.0106236
C -0.9692801 -3.0869585 -0.0648344
H -2.6390367 -1.6980016 -0.0649894
H 0.8465483 -4.2369910 -0.0698080
H -1.6068080 -3.9651938 -0.0935860

2x-H_vac
E(TPSS-D3/def2-TZVP) = -553.8883268717 (conv)
Lowest Freq. = 59.55 cm^-1
27
2x-H_vac (003-H/c1/tpss-d3.def2-TZVP)
C -0.7060843 -0.7194658 -0.0017716
C 0.6853999 -0.8746930 0.0508558
N -0.9696519 0.6614831 0.0638888
N 1.2321945 0.4181930 0.1004606
C 0.2158027 1.3211851 0.1150121
N 0.3951107 2.6524264 0.1857688
C -2.3068108 1.2286023 0.2698078
H -2.8046587 1.4171042 -0.6842380
H -2.2246480 2.1510385 0.8428115
H -2.8875822 0.5082124 0.8477144
C 2.6568006 0.7456843 0.0754578
H 2.8116117 1.6515310 -0.5160188
H 3.1868757 -0.0750275 -0.4077826
H 3.0457135 0.8828946 1.0885815
C -0.4692871 3.6773604 -0.4280874
H 0.1720953 4.4274973 -0.8942478
H -1.1043355 4.1638441 0.3162678
H -1.0851813 3.2223590 -1.2043986
C 1.2834784 -2.1291706 0.0344526
C -1.5624666 -1.8111777 -0.0812150
C 0.4268483 -3.2280481 -0.0458472
H 2.3590195 -2.2581037 0.0841307
C -0.9657726 -3.0727916 -0.1011146
H -2.6398902 -1.6980024 -0.1301781

H 0.8508679 -4.2262493 -0.0645358
H -1.5962930 -3.9533313 -0.1614537
H 1.3159303 2.9556353 0.4731487

2x-CO2_solv
E(TPSS-D3/def2-TZVP) = -742.2029456933 (conv)
Lowest Freq. = 50.30 cm^-1
29
2x-CO2_solv (003-CO2/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -2.0186685 0.6308520 -0.4874038
C -0.6851606 1.0525155 -0.6369175
N -2.7466903 1.7459945 -0.0778475
N -0.6601307 2.4159583 -0.3565796
C -1.9095631 2.8182829 -0.0074381
N -2.2678170 4.0818100 0.3230666
C -4.1498754 1.7376973 0.3360312
H -4.8069876 1.8594648 -0.5278289
H -4.3062282 2.5497044 1.0452896
H -4.3550010 0.7851548 0.8259308
C 0.5027817 3.2887127 -0.4929877
H 0.1493858 4.3053241 -0.6640422
H 1.0840108 2.9485051 -1.3514360
H 1.1020801 3.2586917 0.4179175
C -3.4147187 4.7272018 -0.3398330
H -3.0961410 5.7096032 -0.6937279
H -4.2545827 4.8530358 0.3482585
H -3.7221052 4.1208762 -1.1938943
C 0.3220417 0.1695477 -1.0194074
C -2.4001285 -0.6885326 -0.7174797
C -0.0587469 -1.1525693 -1.2512925
H 1.3517662 0.4905459 -1.1321914
C -1.3918291 -1.5738111 -1.1007409
H -3.4281973 -1.0152235 -0.6052516
H 0.6941261 -1.8732934 -1.5545109
H -1.6442314 -2.6128313 -1.2874280
C -1.5894064 4.7803985 1.4399155
O -1.9763487 5.9550428 1.6113672
O -0.7468671 4.0913272 2.0581121

2y_solv
E(TPSS-D3/def2-TZVP) = -789.4957953979 (conv)
Lowest Freq. = 37.28 cm^-1
44
2y_solv (025/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -0.3193042 -0.8506505 -0.6566015
C 1.0350359 -0.5528772 -0.3753959
N -1.1100448 0.2621609 -0.3077069
N 1.0804196 0.7521219 0.1353951
C -0.1993252 1.3309267 -0.0577119
N -0.3790016 2.5971819 -0.1287606
C -2.3852275 0.0546280 0.5077119
C -3.5896755 -0.0056210 -0.4402874
C -2.2785107 -1.2572252 1.3106590
C 2.2723012 1.5705807 0.5338951
C 2.6939262 2.4787685 -0.6339422
C 3.4531003 0.6725250 0.9353961
C -1.5925222 3.1581570 -0.6960671
H -1.2954149 3.8718738 -1.4756948
H -2.1606469 3.7282069 0.0494876
H -2.2591889 2.4110346 -1.1468646
C 2.0188152 -1.5024258 -0.6680978
C -0.6982600 -2.0551538 -1.2349475
C 1.6281285 -2.7265351 -1.2297888
H 3.0673989 -1.3223343 -0.4878084
C 0.2918033 -3.0061199 -1.5146712
H -1.7363635 -2.2547551 -1.4773103
H 2.3958155 -3.4596533 -1.4614506
H 0.0142685 -3.9534057 -1.9673401

H -2.2622267 -2.1440589 0.6761654
H -3.1521292 -1.3260880 1.9657271
H -1.3771893 -1.2565018 1.9321966
H 3.9704762 0.2526150 0.0707022
H 3.1384397 -0.1356910 1.6021236
H 4.1724479 1.2969935 1.4732664
H -3.4791261 -0.8200267 -1.1624114
H -3.7031174 0.9322461 -0.9915094
H -4.5046953 -0.1807184 0.1356749
H 1.8816281 3.1592030 -0.8965061
H 2.9541450 1.8722874 -1.5083810
H 3.5748485 3.0618847 -0.3440099
C 1.8985279 2.3945884 1.7805796
H 1.0515378 3.0501798 1.5806510
H 2.7635766 2.9991613 2.0712266
H 1.6499721 1.7237665 2.6103830
C -2.5622638 1.1771023 1.5398404
H -1.6805407 1.2638650 2.1817520
H -3.4184685 0.9147781 2.1683951
H -2.7684794 2.1441527 1.0865371

2y_vac
E(TPSS-D3/def2-TZVP) = -789.4879480158 (conv)
Lowest Freq. = 31.98 cm^-1
44
2y_vac (025/c1/tpss-d3.def2-TZVP)
C -0.3191028 -0.8539299 -0.6539448
C 1.0320274 -0.5619337 -0.3587256
N -1.1113473 0.2586445 -0.3028842
N 1.0762996 0.7418066 0.1606547
C -0.2010508 1.3250178 -0.0380002
N -0.3733525 2.5907674 -0.0916797
C -2.3860419 0.0471829 0.5000476
C -3.5833137 -0.0176226 -0.4582316
C -2.2820051 -1.2627982 1.3075814
C 2.2683182 1.5705894 0.5306808
C 2.6662089 2.4713975 -0.6515223
C 3.4603829 0.6819185 0.9202622
C -1.5690440 3.1784667 -0.6575375
H -1.2545774 3.8985717 -1.4241725
H -2.1298831 3.7496632 0.0934815
H -2.2468014 2.4505102 -1.1254278
C 2.0128130 -1.5161007 -0.6410700
C -0.6949527 -2.0531535 -1.2428701
C 1.6240370 -2.7352764 -1.2105696
H 3.0592735 -1.3429434 -0.4443831
C 0.2922866 -3.0070790 -1.5138658
H -1.7306991 -2.2437486 -1.5020874
H 2.3903652 -3.4717119 -1.4341733
H 0.0170222 -3.9505096 -1.9748739
H -2.2397747 -2.1506367 0.6761394
H -3.1652994 -1.3431343 1.9487836
H -1.3910191 -1.2523132 1.9431425
H 3.9672457 0.2610404 0.0495626
H 3.1609264 -0.1261751 1.5939307
H 4.1848922 1.3114647 1.4452590
H -3.4650509 -0.8316358 -1.1790727
H -3.6891636 0.9183575 -1.0137893
H -4.5060030 -0.1916667 0.1062766
H 1.8517783 3.1550816 -0.8961206
H 2.9013153 1.8599930 -1.5294199
H 3.5570751 3.0518575 -0.3868346
C 1.9122817 2.4068810 1.7748890
H 1.0647987 3.0624795 1.5787119
H 2.7814013 3.0137156 2.0492829
H 1.6753473 1.7447725 2.6151873
C -2.5824821 1.1713822 1.5274896
H -1.7047859 1.2753705 2.1715859

H -3.4382375 0.9029875 2.1546406
H -2.7972182 2.1335973 1.0681672

2y-H_vac
E(TPSS-D3/def2-TZVP) = -789.9044820922 (conv)
Lowest Freq. = 44.80 cm^-1
45
2y-H_vac (025-H/c1/tpss-d3.def2-TZVP)
C -0.2790953 -0.9530232 -0.3762757
C 1.0813402 -0.6195152 -0.2225132
N -1.0425858 0.1607311 0.0249619
N 1.1218207 0.7374122 0.1797798
C -0.1719792 1.1753404 0.2741488
N -0.5551784 2.4558824 0.5238901
C -2.5176951 0.0429284 0.4386909
C -3.3711440 -0.0675942 -0.8306817
C -2.6425924 -1.2044558 1.3366528
C 2.3240154 1.6450370 0.4205803
C 2.3018176 2.8124787 -0.5848889
C 3.6416648 0.8922786 0.2045869
C -1.3040753 3.2218017 -0.4979204
H -0.6155763 3.7309919 -1.1825173
H -1.9386482 3.9576383 -0.0013999
H -1.9260332 2.5393481 -1.0747513
C 2.0692436 -1.5719982 -0.5026429
C -0.6756678 -2.1934458 -0.8793462
C 1.6642827 -2.8163486 -0.9733929
H 3.1214497 -1.3763114 -0.3841897
C 0.3137777 -3.1220177 -1.1753416
H -1.7152208 -2.4343390 -1.0527645
H 2.4226905 -3.5570399 -1.2041019
H 0.0319020 -4.0919776 -1.5706292
H -2.3912043 -2.1364884 0.8347029
H -3.6802672 -1.2736444 1.6722997
H -2.0037222 -1.1019697 2.2187735
H 3.7545566 0.5478438 -0.8251738
H 3.7568019 0.0580554 0.8993136
H 4.4475093 1.6022598 0.4068367
H -3.0736697 -0.9082194 -1.4602077
H -3.3063550 0.8458064 -1.4295033
H -4.4169084 -0.2097743 -0.5444354
H 1.4868002 3.5207757 -0.4308332
H 2.2407271 2.4301485 -1.6076142
H 3.2371456 3.3693279 -0.4844859
C 2.3082089 2.1076501 1.8892406
H 1.4332292 2.6998902 2.1734998
H 3.1882302 2.7302808 2.0709743
H 2.3535814 1.2432089 2.5573812
C -2.9953462 1.2255832 1.2924656
H -2.3571382 1.3880647 2.1628060
H -3.9928737 0.9567055 1.6506829
H -3.0945500 2.1560238 0.7368955
H 0.1607434 3.0052160 0.9806403

2y-CO2_solv
E(TPSS-D3/def2-TZVP) = -978.2149675380 (conv)
Lowest Freq. = 40.67 cm^-1
47
2y-CO2_solv (025-CO2/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -0.1699929 -0.9459014 0.0168484
C 1.1827190 -0.5543915 0.0020195
N -0.9340745 0.2201570 0.1434618
N 1.2082345 0.8403510 0.1189736
C -0.0805716 1.2844391 0.1891148
N -0.4619198 2.6013759 0.1841610
C -2.4506732 0.1961984 0.2750970
C -3.0232571 -0.3665319 -1.0356838
C -2.7868655 -0.6672664 1.5047377

C 2.5056056 1.6309949 0.2170342
C 2.3049460 3.1325765 0.4512797
C 3.2630859 1.4491753 -1.1080791
C -0.6760928 3.2799483 -1.0941783
H -0.9731943 4.2991279 -0.8441788
H -1.4683942 2.7978344 -1.6780454
H 0.2385494 3.3003988 -1.6975975
C 2.2041347 -1.5027465 -0.1375317
C -0.5296625 -2.2938016 -0.1088568
C 1.8383277 -2.8374395 -0.2571013
H 3.2491140 -1.2296801 -0.1627476
C 0.4898546 -3.2276156 -0.2432277
H -1.5594019 -2.6209342 -0.1129250
H 2.6140014 -3.5882366 -0.3689335
H 0.2329176 -4.2771392 -0.3447195
H -2.4299697 -1.6938115 1.4270372
H -3.8742829 -0.6929495 1.6169001
H -2.3542787 -0.2127508 2.4008352
H 2.6853337 1.8806987 -1.9312148
H 3.4716139 0.4047982 -1.3428529
H 4.2163479 1.9806365 -1.0386372
H -2.6471821 -1.3618243 -1.2752480
H -2.7834420 0.3037557 -1.8666963
H -4.1111760 -0.4258501 -0.9416932
H 1.7868154 3.3324205 1.3895452
H 1.7955900 3.6303624 -0.3733671
H 3.3115964 3.5562466 0.5227144
C 3.2755828 1.0914552 1.4362836
H 2.6849385 1.2527145 2.3428287
H 4.2106940 1.6512011 1.5248390
H 3.5204410 0.0321861 1.3629869
C -3.0773890 1.5737283 0.5192735
H -2.7237719 2.0227183 1.4478142
H -4.1527451 1.3946399 0.6170954
H -2.9325620 2.2637323 -0.3114719
C -0.6321064 3.2454842 1.4683468
O -0.9802676 4.4465529 1.4511666
O -0.3987896 2.4830040 2.4462245

3a_solv
E(TPSS-D3/def2-TZVP) = -635.7495385858 (conv)
Lowest Freq. = 25.72 cm^-1
38
3a_solv (005/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -2.2086859 0.9202809 -0.6164303
C -0.9310057 1.3337462 -0.5598074
N -3.0614609 1.9850222 -0.2231731
N -0.9050618 2.6654143 -0.1405967
C -2.2253664 3.1285333 -0.0302331
N -2.5013157 4.3867277 0.0784764
C -4.1551193 1.5618882 0.7493781
C 0.3055559 3.5349624 -0.1218993
C -3.7796698 4.9287914 -0.3442080
H -3.5795220 5.8274506 -0.9445746
H -4.4085807 5.2462406 0.4974562
H -4.3665631 4.2291817 -0.9583555
H -2.5990211 -0.0539666 -0.8605632
H -0.0294187 0.7985584 -0.8052932
C 1.5573741 2.6555802 -0.2372944
H 1.6210051 2.1593124 -1.2108125
H 1.5888051 1.8983026 0.5532277
H 2.4361250 3.2981144 -0.1299799
C 0.2606395 4.5155725 -1.3077374
H 1.1542657 5.1486604 -1.2925248
H -0.6296697 5.1438948 -1.2411889
H 0.2421758 3.9630848 -2.2535524
C 0.3538131 4.2863852 1.2183470
H -0.5459340 4.8913795 1.3435181

H 1.2351316 4.9360664 1.2383142
H 0.4272151 3.5737087 2.0471074
C -5.1123776 0.6317737 -0.0080980
H -5.5430774 1.1514959 -0.8696349
H -5.9248968 0.3310747 0.6611464
H -4.6154752 -0.2777679 -0.3575783
C -4.9525894 2.7390085 1.3074627
H -5.6480147 2.3395418 2.0523565
H -5.5363557 3.2394928 0.5338907
H -4.3024797 3.4648569 1.8019183
C -3.4991699 0.8247723 1.9337968
H -2.8067063 1.4917912 2.4588883
H -2.9464292 -0.0570761 1.5990368
H -4.2720794 0.5042530 2.6399045

3a_vac
E(TPSS-D3/def2-TZVP) = -635.7422083735 (conv)
Lowest Freq. = 29.70 cm^-1
38
3a_vac (005/c1/tpss-d3.def2-TZVP)
C -2.2257098 0.9199979 -0.6568526
C -0.9479608 1.3290960 -0.5904689
N -3.0791620 1.9807226 -0.2534979
N -0.9162102 2.6535516 -0.1529990
C -2.2373978 3.1249486 -0.0536758
N -2.4981841 4.3795720 0.0593610
C -4.1440942 1.5596146 0.7434266
C 0.2908685 3.5235576 -0.1171175
C -3.7657764 4.9566381 -0.3332367
H -3.5521390 5.8615262 -0.9177092
H -4.3712345 5.2745699 0.5254700
H -4.3776571 4.2828877 -0.9524955
H -2.6169051 -0.0452164 -0.9318000
H -0.0482798 0.7967630 -0.8475369
C 1.5440412 2.6441900 -0.2186112
H 1.6259048 2.1567735 -1.1956645
H 1.5616774 1.8796723 0.5655302
H 2.4231378 3.2823386 -0.0906881
C 0.2606774 4.5103008 -1.2985931
H 1.1596133 5.1360522 -1.2775862
H -0.6230177 5.1466913 -1.2304409
H 0.2396031 3.9644216 -2.2480413
C 0.3199116 4.2733050 1.2250851
H -0.5811546 4.8786794 1.3354266
H 1.2010148 4.9230326 1.2597954
H 0.3806952 3.5602730 2.0545670
C -5.1004007 0.5998441 0.0216020
H -5.5371210 1.0881032 -0.8545821
H -5.9082323 0.3126903 0.7025529
H -4.6001939 -0.3175610 -0.3018971
C -4.9503642 2.7382768 1.2854098
H -5.6435108 2.3494062 2.0384022
H -5.5360405 3.2244261 0.5038208
H -4.3033503 3.4757363 1.7653937
C -3.4618279 0.8575637 1.9345458
H -2.7818446 1.5499250 2.4420004
H -2.8860546 -0.0121971 1.6070566
H -4.2172614 0.5259370 2.6547382

3a-H_vac
E(TPSS-D3/def2-TZVP) = -636.1722103192 (conv)
Lowest Freq. = 41.25 cm^-1
39
3a-H_vac (005-H/c1/tpss-d3.def2-TZVP)
C -1.7878627 0.7484345 0.4581387
C -0.5868273 1.3210975 0.2099736
N -2.7410556 1.7566499 0.5359167
N -0.7901992 2.6886591 0.0897548

C -2.1169705 2.9447529 0.2908872
N -2.6787868 4.1917544 0.3069906
C -4.1965621 1.4934537 0.9023701
C 0.2958007 3.6986143 -0.2353832
C -3.6684385 4.6448556 -0.6969123
H -3.4608354 4.2300731 -1.6884400
H -3.6041099 5.7325895 -0.7453169
H -4.6829936 4.3809747 -0.3935185
H -2.0378659 -0.2874024 0.5970658
H 0.3830080 0.8694401 0.1071493
C 1.6022375 2.9354934 -0.4887427
H 1.5099227 2.2376546 -1.3257745
H 1.9426300 2.3986189 0.4014622
H 2.3709943 3.6672270 -0.7473565
C -0.0861145 4.4595334 -1.5150698
H 0.7385251 5.1248377 -1.7838518
H -0.9803402 5.0737854 -1.3961948
H -0.2473921 3.7621413 -2.3418526
C 0.5030733 4.6327316 0.9682116
H -0.3460739 5.2955465 1.1649396
H 1.3638194 5.2767203 0.7692593
H 0.7048151 4.0569209 1.8753973
C -5.0307208 1.4531898 -0.3858674
H -5.0125234 2.4010695 -0.9245838
H -6.0699788 1.2292772 -0.1296965
H -4.6658502 0.6668149 -1.0530532
C -4.6815499 2.5523319 1.9014050
H -5.6997922 2.2894586 2.1994457
H -4.6972370 3.5603779 1.4911734
H -4.0528309 2.5529768 2.7965127
C -4.2738567 0.1210833 1.5890853
H -3.6111034 0.0642955 2.4573385
H -4.0524601 -0.7017645 0.9037454
H -5.3004371 -0.0162637 1.9367220
H -1.9941732 4.9032078 0.5245426

3a-CO2_solv
E(TPSS-D3/def2-TZVP) = -824.4827626003 (conv)
Lowest Freq. = 24.40 cm^-1
41
3a-CO2_solv (005-CO2/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -2.0123879 0.8665551 -0.4321654
C -0.7859888 1.4017169 -0.6655706
N -2.8000093 1.8540896 0.1275195
N -0.8083207 2.7134052 -0.2313335
C -2.0561698 2.9932019 0.2441986
N -2.4941758 4.1962372 0.7330661
C -4.2291191 1.6303571 0.5822790
C 0.3775015 3.6389056 -0.4250675
C -2.5012591 4.4808563 2.1716638
H -1.9922365 5.4301926 2.3558244
H -1.9739002 3.6813391 2.6962227
H -3.5249924 4.5533731 2.5559651
H -2.3713542 -0.1299355 -0.6178253
H 0.0869236 0.9504466 -1.1034359
C 1.6490949 2.8279621 -0.1294847
H 1.8077856 2.0219858 -0.8500289
H 1.6202980 2.4071297 0.8802400
H 2.5041908 3.5052871 -0.1997005
C 0.3524554 4.1087377 -1.8861727
H 1.1991132 4.7801353 -2.0588455
H -0.5813859 4.6381497 -2.0918496
H 0.4408650 3.2566338 -2.5677944
C 0.3351226 4.8347563 0.5323712
H -0.4588778 5.5406695 0.2900878
H 1.2926657 5.3545038 0.4346103
H 0.2311353 4.5120988 1.5717797
C -4.7823273 0.4174783 -0.1790496

H -4.7195510 0.5638047 -1.2615670
H -5.8345742 0.3068230 0.0938904
H -4.2715634 -0.5103632 0.0922665
C -5.1012187 2.8520685 0.2597476
H -6.1455390 2.5578007 0.3977223
H -4.9582448 3.1710753 -0.7756943
H -4.8974247 3.6947489 0.9205929
C -4.2083698 1.3346651 2.0882185
H -3.8331038 2.1889273 2.6555497
H -3.5826788 0.4628475 2.3023203
H -5.2284499 1.1222918 2.4218751
C -2.9385775 5.1970495 -0.2147192
O -3.3116706 6.2812947 0.2938109
O -2.8915732 4.8443118 -1.4222586

3a-CO2-TS_solv
E(TPSS-D3/def2-TZVP) = -824.4275072492 (conv)
Lowest Freq. = -270.58 cm^-1
41
3a-CO2-TS_solv (005-CO2_TS1/c1b/tpss-d3.def2-TZVP_COSMO_37.5)
C 0.0661536 -2.0783048 -0.3340509
C 1.3098227 -1.5761692 -0.4382988
N -0.8412441 -1.0046155 -0.2879509
N 1.2201813 -0.1761360 -0.4180962
C -0.1083357 0.1734255 -0.1925446
N -0.4116648 1.1430565 1.2491001
C -2.2831899 -1.2157718 0.0571193
C 2.3325138 0.7421238 -0.8234261
C -0.0734884 1.2853654 2.6492917
H 0.0462271 2.3446823 2.9034338
H 0.8728196 0.7695649 2.8475648
H -0.8445692 0.8505579 3.2961688
H -0.2619677 -3.1022142 -0.2900891
H 2.2521421 -2.0867427 -0.5279032
C 3.6627153 -0.0005133 -0.6249912
H 3.7635852 -0.8502221 -1.3060885
H 3.7714621 -0.3513425 0.4061761
H 4.4768108 0.6965994 -0.8407318
C 2.1673740 1.1089734 -2.3090785
H 3.0078647 1.7343104 -2.6285585
H 1.2381390 1.6597568 -2.4705558
H 2.1554836 0.2027821 -2.9235386
C 2.3605005 2.0088484 0.0448041
H 1.5037197 2.6589834 -0.1389231
H 3.2622408 2.5731871 -0.2116421
H 2.4030984 1.7578054 1.1080115
C -2.7961545 -2.3864486 -0.7988437
H -2.6522715 -2.1777694 -1.8634995
H -3.8655210 -2.5152420 -0.6084219
H -2.3001430 -3.3291624 -0.5527201
C -3.1351512 0.0179832 -0.2669928
H -4.1824884 -0.2520292 -0.1005580
H -3.0149089 0.3239266 -1.3088500
H -2.9009644 0.8603947 0.3860059
C -2.3993750 -1.5613438 1.5513590
H -2.0560222 -0.7262996 2.1662989
H -1.8015840 -2.4467010 1.7907871
H -3.4445977 -1.7705708 1.8007848
C -0.7628987 2.0923848 0.3947724
O -1.1140658 3.2620912 0.4332570
O -0.6145743 1.3522477 -0.8213676

Imidazolinone
E(TPSS-D3/def2-TZVP) = -616.3561965848 (conv)
Lowest Freq. = 51.36 cm^-1
34
Imidazolinone (028/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C 0.0648691 -2.1754900 -0.6030748

C 1.2975920 -1.6541717 -0.8086540
N -0.8015940 -1.1229694 -0.3058671
N 1.2115792 -0.2715476 -0.6417549
C -0.0973131 0.0757253 -0.3263712
C -2.2604805 -1.2212598 -0.0059964
C 2.3226395 0.7169955 -0.7690537
H -0.2620842 -3.2000558 -0.6443101
H 2.2193806 -2.1506417 -1.0580967
C 3.6160750 -0.0224429 -1.1251578
H 3.5295724 -0.5481320 -2.0814830
H 3.8987291 -0.7383733 -0.3468018
H 4.4178800 0.7159530 -1.2147840
C 1.9734178 1.7107876 -1.8890769
H 2.7780144 2.4468285 -1.9868438
H 1.0408018 2.2313466 -1.6611632
H 1.8652333 1.1838023 -2.8428985
C 2.4966669 1.4393398 0.5771229
H 1.5747225 1.9538543 0.8566857
H 3.3040849 2.1740669 0.4948033
H 2.7574344 0.7209264 1.3613553
C -2.6903271 -2.6900303 -0.0726763
H -2.5282322 -3.1127650 -1.0693393
H -3.7600116 -2.7429443 0.1488769
H -2.1596017 -3.2993192 0.6658226
C -3.0359833 -0.4100026 -1.0570027
H -4.1081557 -0.4672917 -0.8431642
H -2.8576066 -0.8180276 -2.0574682
H -2.7249033 0.6367267 -1.0378212
C -2.5110468 -0.6757638 1.4095278
H -2.1889112 0.3654090 1.4805551
H -1.9628541 -1.2710779 2.1473043
H -3.5799532 -0.7346036 1.6387369
O -0.5443181 1.2188979 -0.1083068

Me-NCO
E(TPSS-D3/def2-TZVP) = -208.1194066939 (conv)
Lowest Freq. = 83.67 cm^-1
7
Me-NCO (029/c1/tpss-d3.def2-TZVP_COSMO_37.5)
N -0.2866284 1.5189867 1.3321505
C -0.0634613 1.2390548 2.7405562
H 0.4622234 2.0746621 3.2099459
H 0.5460463 0.3383065 2.8197932
H -1.0193763 1.0743431 3.2446877
C -0.8237931 2.3258720 0.6245824
O -1.3049446 3.0400518 -0.1928790

3b_solv
E(TPSS-D3/def2-TZVP) = -753.7540385664 (conv)
Lowest Freq. = 34.30 cm^-1
47
3b_solv (015/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -2.1747469 0.8779225 -0.6756014
C -0.9116665 1.3362647 -0.6205415
N -3.0506895 1.8803051 -0.1899920
N -0.9248407 2.6428514 -0.1317149
C -2.2650315 3.0633209 0.0053405
N -2.5769082 4.3014398 0.1819900
C -4.0405360 1.3613299 0.8492407
C 0.2729097 3.5225227 -0.0307299
C -3.7347145 5.0315282 -0.3584244
C -3.1167970 6.1573338 -1.2267162
C -4.5150262 5.7309084 0.7710401
C -4.6680596 4.2317046 -1.2862858
H -2.5370964 -0.0938463 -0.9710771
H 0.0030011 0.8525689 -0.9194662
C 1.5392898 2.6589442 -0.1079978

H 1.6663103 2.2022171 -1.0945941
H 1.5323178 1.8707802 0.6523302
H 2.4032646 3.3044516 0.0755704
C 0.2767909 4.5396860 -1.1840495
H 1.1753106 5.1633110 -1.1204384
H -0.6070637 5.1747216 -1.1231734
H 0.2814246 4.0201101 -2.1484617
C 0.2468856 4.2386232 1.3286938
H -0.6654718 4.8317650 1.4121635
H 1.1218229 4.8922700 1.4106726
H 0.2802116 3.5063643 2.1429783
C -5.1168290 0.5629133 0.1041308
H -5.6619192 1.2091663 -0.5905286
H -5.8280085 0.1444817 0.8242599
H -4.6815418 -0.2675167 -0.4606907
C -4.6878308 2.4788315 1.6621240
H -5.2537614 2.0142789 2.4755273
H -5.3843565 3.0702288 1.0696080
H -3.9362706 3.1432010 2.0940120
C -3.2869865 0.4512166 1.8428560
H -2.4712522 1.0041697 2.3210833
H -2.8669511 -0.4291113 1.3506341
H -3.9803782 0.1150242 2.6205468
H -2.5766273 5.7277794 -2.0769479
H -2.4136144 6.7453407 -0.6284012
H -3.8995783 6.8228107 -1.6113414
H -4.0899526 3.7814113 -2.0999538
H -5.4081551 4.9118555 -1.7240565
H -5.2043441 3.4307970 -0.7773015
H -5.2621982 6.4108053 0.3450780
H -3.8198110 6.3190432 1.3803157
H -5.0289744 5.0254538 1.4253297

3b_vac
E(TPSS-D3/def2-TZVP) = -753.7481630991 (conv)
Lowest Freq. = 32.66 cm^-1
47
3b_vac (015/c1/tpss-d3.def2-TZVP)
C -2.1927902 0.8850054 -0.7236291
C -0.9290980 1.3350841 -0.6483925
N -3.0715672 1.8839737 -0.2303113
N -0.9359696 2.6342165 -0.1380583
C -2.2771829 3.0654605 -0.0307783
N -2.5780955 4.3039063 0.1197575
C -4.0201675 1.3647286 0.8444533
C 0.2586486 3.5102598 -0.0066519
C -3.7450269 5.0383107 -0.3891954
C -3.1362815 6.1569984 -1.2721792
C -4.4881020 5.7421440 0.7621962
C -4.7065011 4.2424099 -1.2912578
H -2.5572658 -0.0755945 -1.0501590
H -0.0150490 0.8537307 -0.9518656
C 1.5239583 2.6441669 -0.0772627
H 1.6697481 2.2088059 -1.0712818
H 1.5002338 1.8396183 0.6653797
H 2.3881288 3.2798740 0.1362908
C 0.2860952 4.5462497 -1.1434122
H 1.1898900 5.1600950 -1.0610894
H -0.5905248 5.1905684 -1.0834075
H 0.2962624 4.0430262 -2.1163435
C 0.2122054 4.2029968 1.3652862
H -0.7026476 4.7906694 1.4566862
H 1.0807842 4.8620619 1.4696513
H 0.2438811 3.4567047 2.1666349
C -5.1112029 0.5516304 0.1372252
H -5.6718871 1.1855709 -0.5555698
H -5.8054592 0.1390016 0.8772047
H -4.6868014 -0.2850050 -0.4267031

C -4.6543398 2.4862362 1.6631591
H -5.2023614 2.0283060 2.4927649
H -5.3639217 3.0717101 1.0803315
H -3.8971552 3.1572063 2.0744405
C -3.2325739 0.4713096 1.8267359
H -2.4106202 1.0362720 2.2785708
H -2.8126541 -0.4073743 1.3319641
H -3.8999462 0.1327442 2.6261730
H -2.6084757 5.7216032 -2.1268536
H -2.4248049 6.7474640 -0.6870798
H -3.9217293 6.8222427 -1.6506010
H -4.1549372 3.7824691 -2.1171293
H -5.4522984 4.9261122 -1.7130464
H -5.2368659 3.4475752 -0.7666021
H -5.2336849 6.4362447 0.3575409
H -3.7707621 6.3134336 1.3601501
H -4.9995349 5.0413560 1.4233039

3b-H_vac
E(TPSS-D3/def2-TZVP) = -754.1807360330 (conv)
Lowest Freq. = 25.42 cm^-1
48
3b-H_vac (015-H/c1/tpss-d3.def2-TZVP)
C -2.0797083 0.8510777 -0.3760471
C -0.8701218 1.4028229 -0.6129587
N -2.9055162 1.8308470 0.1634003
N -0.9392051 2.7488473 -0.2777448
C -2.2226931 3.0164928 0.1534534
N -2.7454932 4.2381186 0.4700331
C -4.1054368 1.3598108 1.0025353
C 0.2993349 3.6233577 -0.1237376
C -3.7386418 5.0116690 -0.4135130
C -2.9706677 6.0089476 -1.2935553
C -4.6564540 5.7985995 0.5286820
C -4.5140414 4.0686547 -1.3298570
H -2.4171110 -0.1600256 -0.5227300
H 0.0258227 0.9515063 -0.9981234
C 1.5194391 2.8284354 -0.6068407
H 1.4413453 2.5639831 -1.6655973
H 1.6866384 1.9255809 -0.0131258
H 2.3969224 3.4683606 -0.4882507
C 0.1909161 4.9010932 -0.9597492
H 1.1579798 5.4105068 -0.9352158
H -0.5532636 5.5940903 -0.5708944
H -0.0477852 4.6708694 -2.0013609
C 0.4694778 3.9341263 1.3721495
H -0.3571612 4.5254680 1.7786731
H 1.3853926 4.5137610 1.5150056
H 0.5498397 3.0107872 1.9527023
C -5.1018343 0.6636007 0.0697570
H -5.5064608 1.3510890 -0.6761974
H -5.9317414 0.2789629 0.6689249
H -4.6481265 -0.1846369 -0.4506656
C -4.7735903 2.4889080 1.7807756
H -5.5178625 2.0245392 2.4337638
H -5.2963533 3.1914022 1.1357536
H -4.0634508 3.0359203 2.4023971
C -3.5321024 0.3595003 2.0269345
H -2.7735569 0.8381890 2.6533338
H -3.0924339 -0.5192491 1.5503111
H -4.3466174 0.0196067 2.6718269
H -2.3236474 5.5004765 -2.0120355
H -2.3704982 6.6981290 -0.6892618
H -3.6903360 6.6123402 -1.8548545
H -3.8426614 3.5000701 -1.9813113
H -5.1645968 4.6731385 -1.9672492
H -5.1468755 3.3708350 -0.7825185
H -5.3423607 6.4151017 -0.0597253

H -4.0677150 6.4672619 1.1657005
H -5.2456675 5.1464444 1.1742293
H -2.0400395 4.8754878 0.8253275

3b-CO2_solv
E(TPSS-D3/def2-TZVP) = -942.4853066712 (conv)
Lowest Freq. = 31.63 cm^-1
50
3b-CO2_solv (015-CO2/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -2.0048608 0.8860027 -0.2408831
C -0.7738195 1.4033571 -0.4569648
N -2.8097682 1.8992951 0.2448572
N -0.8039302 2.7364325 -0.0942731
C -2.0597264 3.0453133 0.3634584
N -2.4765645 4.2489119 0.9000444
C -4.2906175 1.6416297 0.4862579
C 0.3622236 3.6179577 -0.5156267
C -2.3940095 4.5319779 2.3945054
H -2.3631445 -0.1157801 -0.3950364
H 0.1085061 0.9325805 -0.8535348
C 1.6566228 2.9349975 -0.0479387
H 1.8272473 1.9728929 -0.5367746
H 1.6470658 2.7871601 1.0362423
H 2.4960861 3.5882842 -0.3012778
C 0.2943903 3.7079163 -2.0487300
H 1.1253543 4.3244900 -2.4043469
H -0.6510619 4.1682421 -2.3476381
H 0.3762111 2.7182512 -2.5081108
C 0.3123564 5.0168824 0.0838744
H -0.5848095 5.5624650 -0.2033634
H 1.1833772 5.5567540 -0.2996193
H 0.3951687 4.9797779 1.1697384
C -4.7641288 0.6298659 -0.5750034
H -4.5219209 0.9757807 -1.5840303
H -5.8506026 0.5470611 -0.4881991
H -4.3466712 -0.3684205 -0.4235176
C -5.1247490 2.9118221 0.2980826
H -6.1761210 2.6235152 0.3872698
H -4.9576567 3.3326975 -0.6960787
H -4.9180373 3.6762559 1.0410119
C -4.4505671 1.0239166 1.8807936
H -4.1140194 1.7012894 2.6670597
H -3.8784850 0.0938228 1.9548234
H -5.5068563 0.7957379 2.0510228
C -3.0469309 5.1661086 -0.0727347
O -3.5973059 6.2027405 0.3622540
O -2.9119064 4.7819194 -1.2683290
C -1.7366047 5.8986501 2.6622512
H -0.6931486 5.9246549 2.3488469
H -1.7672858 6.0820439 3.7415985
H -2.2850147 6.6903012 2.1511279
C -3.7929960 4.5681492 3.0333782
H -4.4220638 5.2961159 2.5153777
H -3.6946817 4.8725153 4.0807340
H -4.2815348 3.5926154 3.0169127
C -1.5473482 3.4362040 3.0533779
H -1.4999205 3.6322160 4.1285867
H -0.5247427 3.4311769 2.6639648
H -1.9777339 2.4399340 2.9125502

3b-CO2-TS_solv
E(TPSS-D3/def2-TZVP) = -942.4448318482 (conv)
Lowest Freq. = -218.89 cm^-1
50
3b-CO2-TS_solv (015-CO2_TS1/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C 0.2391265 -2.0525206 -0.1058058
C 1.4497509 -1.5013916 -0.3039544
N -0.7098870 -1.0204403 -0.0382753

N 1.2976891 -0.1067563 -0.3356889
C -0.0389983 0.1987809 -0.0572535
N -0.3014538 1.2480331 1.3049180
C -2.1659292 -1.3271792 0.1265509
C 2.3080110 0.8102091 -0.9540405
C -0.1172234 1.3697654 2.7594797
H -0.0384902 -3.0854430 0.0201205
H 2.4123400 -1.9723007 -0.3962056
C 3.6975278 0.1777347 -0.7764011
H 3.8076582 -0.7429617 -1.3560392
H 3.9025691 -0.0347827 0.2776951
H 4.4452515 0.8888219 -1.1381496
C 2.0021885 0.9626536 -2.4550645
H 2.7784569 1.5723149 -2.9299756
H 1.0341358 1.4460362 -2.6049367
H 1.9877897 -0.0196434 -2.9388793
C 2.3230335 2.1795818 -0.2634040
H 1.3934054 2.7310728 -0.4081099
H 3.1333996 2.7706921 -0.7011788
H 2.5143322 2.0722002 0.8065383
C -2.5836993 -2.2119878 -1.0615777
H -2.4395445 -1.6740915 -2.0036345
H -3.6416163 -2.4750731 -0.9637818
H -2.0041019 -3.1392663 -1.0955669
C -3.0466600 -0.0730349 0.1320901
H -4.0816585 -0.4052562 0.2569631
H -2.9710495 0.4788882 -0.8061680
H -2.8049187 0.5924613 0.9625378
C -2.3593105 -2.0902000 1.4488309
H -2.0486635 -1.4757277 2.2980162
H -1.7799659 -3.0181721 1.4623540
H -3.4163065 -2.3449707 1.5728432
C -0.8157937 2.0980516 0.4273218
O -1.3158981 3.2118118 0.4132016
O -0.6356681 1.2995356 -0.7527590
C -1.4860841 1.3688886 3.4631741
H -2.0954618 2.2086809 3.1138939
H -1.3516311 1.4642394 4.5462159
H -2.0268297 0.4393754 3.2641002
C 0.6303377 2.6720950 3.0971655
H 0.0752459 3.5405194 2.7304974
H 1.6265020 2.6770121 2.6468909
H 0.7407227 2.7613294 4.1834503
C 0.7142198 0.1550378 3.1975820
H 0.2020443 -0.7786458 2.9456840
H 0.8715762 0.1854010 4.2800063
H 1.6892969 0.1577977 2.7007811

tBu-NCO
E(TPSS-D3/def2-TZVP) = -326.1398767350 (conv)
Lowest Freq. = 15.00 cm^-1
16
tBu-NCO (030/c1/tpss-d3.def2-TZVP_COSMO_37.5)
N -0.3503333 1.4440305 1.3700574
C -0.1215468 1.4312116 2.8338821
C -0.8444423 2.1592966 0.5392290
O -1.2933126 2.7622499 -0.3803158
C -1.4846865 1.3844767 3.5380049
H -2.0695345 2.2798689 3.3045378
H -1.3334929 1.3383810 4.6213142
H -2.0484876 0.5006457 3.2251704
C 0.6562115 2.6965167 3.2206146
H 0.0730168 3.5932328 2.9875566
H 1.6079004 2.7418301 2.6828529
H 0.8618216 2.6836359 4.2958222
C 0.6956130 0.1726941 3.1473085
H 0.1493728 -0.7252372 2.8429005

H 0.8862331 0.1192772 4.2233961
H 1.6552367 0.1972822 2.6220303

3c_solv
E(TPSS-D3/def2-TZVP) = -714.4237213448 (conv)
Lowest Freq. = 28.81 cm^-1
44
3c_solv (016/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C 0.3870036 -2.2054335 -0.2911294
C 1.6572011 -1.7601217 -0.3043476
N -0.4645590 -1.1397113 0.0557444
N 1.6492258 -0.4064578 0.0160180
C 0.3249422 0.0348811 0.1984631
N 0.0674299 1.2915864 0.3881686
C -1.7267650 -1.5221266 0.7881991
C 2.8418458 0.4891940 -0.0211638
C -1.1057587 2.0130230 -0.0755486
H 0.0087161 -3.1973610 -0.4749688
H 2.5636992 -2.2910513 -0.5384391
C 4.1009836 -0.3551760 -0.2558209
H 4.0880001 -0.8453221 -1.2345900
H 4.2292171 -1.1139027 0.5233609
H 4.9665327 0.3129778 -0.2245988
C 2.6947880 1.4995961 -1.1729647
H 3.5779508 2.1467393 -1.2029281
H 1.8011776 2.1082660 -1.0263634
H 2.6177898 0.9715085 -2.1297079
C 2.9724254 1.2027649 1.3342938
H 2.0624768 1.7680080 1.5436157
H 3.8304440 1.8829623 1.3076870
H 3.1341394 0.4687449 2.1315107
C -2.6175704 -2.3127389 -0.1818281
H -2.8847561 -1.6927706 -1.0434317
H -3.5368669 -2.6117697 0.3319912
H -2.1245906 -3.2198733 -0.5434950
C -2.5074235 -0.3184974 1.3094367
H -3.3310689 -0.6994877 1.9209657
H -2.9380555 0.2667806 0.4965923
H -1.8818042 0.3239571 1.9331120
C -1.3344124 -2.3943531 1.9988243
H -0.6797075 -1.8322716 2.6732804
H -0.8150758 -3.3050185 1.6890441
H -2.2368612 -2.6805261 2.5485405
H -0.8014171 3.0672804 -0.1562969
H -1.9355509 2.0107210 0.6471998
C -1.6314655 1.5784588 -1.4527730
H -0.8179514 1.6809278 -2.1822750
C -2.8428467 2.4068360 -1.8904288
H -1.8957973 0.5146181 -1.4325366
H -2.5971381 3.4752753 -1.9232916
H -3.6781029 2.2785652 -1.1909826
H -3.1904435 2.1102982 -2.8861378

3c_vac
E(TPSS-D3/def2-TZVP) = -714.4162110018 (conv)
Lowest Freq. = 29.93 cm^-1
44
3c_vac (016/c1/tpss-d3.def2-TZVP)
C -1.9857418 0.7997941 -0.4270772
C -0.7134430 1.2321291 -0.3929896
N -2.8426229 1.8632183 -0.0708128
N -0.7093352 2.5745046 -0.0277821
C -2.0363109 3.0321342 0.1094724
N -2.2788783 4.2855752 0.2772513
C -4.0496988 1.4698340 0.7400694
C 0.4883868 3.4594530 -0.0060018
C -3.4578213 5.0251364 -0.1239005
H -2.3664920 -0.1807411 -0.6589210

H 0.1921428 0.7016152 -0.6301762
C 1.7490881 2.6015229 -0.1756620
H 1.7907488 2.1234084 -1.1599012
H 1.8204030 1.8317516 0.6002526
H 2.6215162 3.2549017 -0.0845929
C 0.4098341 4.4736024 -1.1616563
H 1.3071835 5.1019763 -1.1578645
H -0.4730402 5.1035081 -1.0464235
H 0.3563950 3.9498361 -2.1222497
C 0.5576140 4.1756008 1.3532081
H -0.3485359 4.7624010 1.5112166
H 1.4304426 4.8373273 1.3722877
H 0.6597509 3.4424815 2.1609133
C -4.9703705 0.6322422 -0.1605174
H -5.2829849 1.2168504 -1.0309755
H -5.8621785 0.3365509 0.4018058
H -4.4818957 -0.2807936 -0.5133792
C -4.8320487 2.6723738 1.2610571
H -5.6371109 2.2964015 1.9005157
H -5.2857790 3.2414966 0.4490328
H -4.1963291 3.3301333 1.8574583
C -3.5791274 0.6446773 1.9557246
H -2.9118780 1.2449881 2.5826116
H -3.0416419 -0.2556853 1.6468526
H -4.4438066 0.3447890 2.5572294
H -3.1474455 6.0779844 -0.1885419
H -4.2587725 5.0121129 0.6299390
C -4.0340638 4.6216065 -1.4911988
H -3.2474702 4.7422931 -2.2464168
C -5.2603153 5.4584341 -1.8652701
H -4.2928473 3.5562781 -1.4881284
H -5.0188122 6.5279225 -1.8779641
H -6.0725911 5.3122658 -1.1426690
H -5.6420362 5.1894770 -2.8561156

3c-H_vac
E(TPSS-D3/def2-TZVP) = -714.8480569696 (conv)
Lowest Freq. = 31.64 cm^-1
45
3c-H_vac (016-H/c1/tpss-d3.def2-TZVP)
C -1.9441792 0.7656241 -0.1115636
C -0.7181406 1.2995019 -0.3213967
N -2.7796695 1.7706352 0.3564488
N -0.7941971 2.6519160 -0.0245711
C -2.0700304 2.9342142 0.3873808
N -2.5283379 4.1597447 0.7802363
C -4.1472434 1.3990310 0.9285160
C 0.3704850 3.6203098 -0.1172774
C -3.4325908 5.0041817 -0.0657303
H -2.2870282 -0.2459274 -0.2415590
H 0.1879718 0.8312457 -0.6607655
C 1.5703314 2.8772004 -0.7182521
H 1.3517452 2.4949898 -1.7195555
H 1.9084752 2.0572895 -0.0779743
H 2.3943330 3.5891859 -0.8049158
C 0.0029321 4.7896233 -1.0424193
H 0.8793058 5.4342451 -1.1494960
H -0.8118779 5.4002813 -0.6512053
H -0.2751066 4.4237943 -2.0346583
C 0.7423450 4.0912303 1.2980054
H -0.0303537 4.7088679 1.7668393
H 1.6465915 4.7032164 1.2417411
H 0.9433247 3.2370619 1.9503455
C -4.9400281 0.7021762 -0.1854841
H -5.0907671 1.3700854 -1.0383451
H -5.9205445 0.4201719 0.2072165
H -4.4494993 -0.2093390 -0.5373507
C -4.9302970 2.6079183 1.4385495

H -5.8484467 2.2221669 1.8899791
H -5.2229948 3.2768506 0.6281590
H -4.3827206 3.1677815 2.1972910
C -3.8766949 0.4419365 2.1021249
H -3.2856249 0.9374407 2.8777629
H -3.3505425 -0.4611845 1.7820995
H -4.8327885 0.1391305 2.5371150
H -2.9390182 5.9761321 -0.1764926
H -4.3627361 5.1763897 0.4843430
C -3.7232619 4.4233277 -1.4454131
H -2.7799366 4.2570210 -1.9790207
C -4.6291831 5.3576825 -2.2541319
H -4.2039747 3.4432981 -1.3457981
H -4.1576957 6.3347878 -2.4013706
H -5.5855545 5.5173436 -1.7452644
H -4.8389708 4.9328985 -3.2392034
H -1.8086825 4.7060686 1.2354560

3c-CO2_solv
E(TPSS-D3/def2-TZVP) = -903.1583987657 (conv)
Lowest Freq. = 27.80 cm^-1
47
3c-CO2_solv (016-CO2/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C 0.3179257 -2.3415580 -0.4300203
C 1.4766751 -1.7176991 -0.7603491
N -0.4944616 -1.4142682 0.1961235
N 1.3844950 -0.4063509 -0.3326548
C 0.1728887 -0.2240340 0.2658139
N -0.2902078 0.9328144 0.8351978
C -1.8027645 -1.8211685 0.8478868
C 2.5720657 0.5269311 -0.4617501
C -1.0439326 1.9454309 0.0698820
H 0.0160615 -3.3612361 -0.5930542
H 2.3480344 -2.1020869 -1.2624377
C 2.9620668 0.5641435 -1.9469448
H 2.1404899 0.9587070 -2.5525518
H 3.2355872 -0.4245659 -2.3246370
H 3.8275725 1.2221211 -2.0635655
C 2.2783166 1.9492228 0.0180429
H 3.1902560 2.5282789 -0.1565367
H 2.0505024 1.9854915 1.0836490
H 1.4721920 2.4196359 -0.5472554
C 3.6941384 -0.0760333 0.3983309
H 3.3745409 -0.1358285 1.4425278
H 4.5749610 0.5690792 0.3326217
H 3.9736764 -1.0750327 0.0519151
C -2.5093550 -2.8023430 -0.0996097
H -2.6738299 -2.3483512 -1.0816100
H -3.4809865 -3.0515316 0.3348522
H -1.9556634 -3.7360132 -0.2245395
C -2.7332522 -0.6289626 1.0902590
H -3.6846862 -1.0369301 1.4436926
H -2.9281759 -0.0773731 0.1673791
H -2.3542419 0.0544114 1.8494719
C -1.4396303 -2.4976762 2.1778998
H -0.8937879 -1.7977743 2.8164052
H -0.8197888 -3.3833823 2.0060496
H -2.3586571 -2.8093465 2.6833352
H -0.5412492 2.9102389 0.2030514
H -2.0433423 2.0418506 0.5106703
C -1.1583160 1.6133864 -1.4161289
H -0.1589495 1.5288172 -1.8596157
C -1.9590878 2.6887112 -2.1567794
H -1.6423488 0.6378413 -1.5478280
H -1.4768380 3.6682079 -2.0633343
H -2.9730711 2.7703336 -1.7493665
H -2.0384811 2.4486666 -3.2214852
C -0.0281412 1.1240690 2.2439846

O 0.6549538 0.2113563 2.7827898
O -0.5089691 2.1688406 2.7444142

3d_solv
E(TPSS-D3/def2-TZVP) = -911.1090582988 (conv)
Lowest Freq. = 11.47 cm^-1
59
3d_solv (017/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -1.6361497 0.6886673 -0.0993105
C -0.3545620 1.0604531 0.0773719
N -2.4721502 1.7779268 0.2105412
N -0.3373133 2.3900071 0.4862759
C -1.6509336 2.8949884 0.5292652
N -1.8679147 4.1514485 0.7648265
C -3.8377554 1.4241926 0.7453254
C 0.8923158 3.2165059 0.6597556
C -2.9442102 4.9589754 0.2144220
H -2.0357966 -0.2666697 -0.3968049
H 0.5473885 0.4936777 -0.0762248
C 2.1283019 2.3168822 0.5321056
H 2.2196831 1.8873790 -0.4706668
H 2.1157607 1.5070538 1.2691401
H 3.0140748 2.9312172 0.7179057
C 0.9463513 4.2996979 -0.4325075
H 1.8552053 4.8978400 -0.3060717
H 0.0707391 4.9469466 -0.3625816
H 0.9716899 3.8338323 -1.4237202
C 0.8802558 3.8402919 2.0648320
H -0.0203708 4.4431457 2.1941662
H 1.7668151 4.4707665 2.1919842
H 0.9007910 3.0525206 2.8259857
C -4.6341248 0.7599141 -0.3879247
H -4.7555388 1.4546207 -1.2251006
H -5.6263695 0.4809828 -0.0189998
H -4.1444233 -0.1468365 -0.7550153
C -4.6165662 2.6335954 1.2565726
H -5.5281068 2.2606627 1.7336864
H -4.9131538 3.2973438 0.4440996
H -4.0427959 3.1942321 1.9979332
C -3.6534447 0.4462136 1.9244215
H -3.0632818 0.9175935 2.7174196
H -3.1475333 -0.4714407 1.6132208
H -4.6338303 0.1794746 2.3319693
H -2.5815201 5.9973417 0.2273945
H -3.8480585 4.9649107 0.8417838
C -3.3322822 4.6203352 -1.2330724
H -2.4486110 4.7502065 -1.8722805
C -4.4841259 5.4871301 -1.7491781
H -3.6117916 3.5620811 -1.3064732
H -4.2088956 6.5488743 -1.6715230
H -5.3612323 5.3465961 -1.1003778
C -4.8756722 5.1697237 -3.1965548
H -4.0026340 5.3159635 -3.8486176
C -6.0404272 6.0227694 -3.7106689
H -5.1449401 4.1061925 -3.2720911
H -5.7712474 7.0862558 -3.6353143
H -6.9121965 5.8758605 -3.0567031
C -6.4348372 5.7029393 -5.1565345
H -5.5640239 5.8516113 -5.8115548
C -7.6025606 6.5534745 -5.6696526
H -6.7020355 4.6387988 -5.2324199
H -7.3340606 7.6161893 -5.5937664
H -8.4713599 6.4045431 -5.0136902
C -7.9898053 6.2247855 -7.1154418
H -7.1448837 6.3936987 -7.7940074
H -8.8258045 6.8454491 -7.4570595
H -8.2890407 5.1738963 -7.2101443

3d_vac
E(TPSS-D3/def2-TZVP) = -911.1008857084 (conv)
Lowest Freq. = 10.59 cm^-1
59
3d_vac (017/c1/tpss-d3.def2-TZVP)
C -1.6164127 0.6822638 -0.1584550
C -0.3420238 1.0434763 0.0706338
N -2.4618635 1.7752883 0.1265391
N -0.3248644 2.3679745 0.4957294
C -1.6344755 2.8911525 0.4699835
N -1.8373144 4.1486460 0.6597248
C -3.7967190 1.4179541 0.7253260
C 0.8989252 3.1860107 0.7215800
C -2.9169900 4.9619191 0.1382634
H -2.0080650 -0.2659335 -0.4866216
H 0.5611973 0.4741510 -0.0629098
C 2.1285669 2.2689765 0.6871570
H 2.2837924 1.8276928 -0.3029166
H 2.0543017 1.4672321 1.4296209
H 3.0100310 2.8706456 0.9264674
C 1.0304209 4.2464434 -0.3867425
H 1.9470089 4.8258860 -0.2309730
H 0.1706482 4.9171022 -0.3657982
H 1.0873182 3.7633551 -1.3682369
C 0.8128331 3.8446140 2.1086686
H -0.0778564 4.4719527 2.1681196
H 1.7048021 4.4579969 2.2765793
H 0.7676096 3.0765535 2.8885533
C -4.6198093 0.6980769 -0.3539062
H -4.7688140 1.3542640 -1.2167757
H -5.5993300 0.4253092 0.0525199
H -4.1338908 -0.2200859 -0.6971900
C -4.5771672 2.6372852 1.2097779
H -5.4814229 2.2778100 1.7113616
H -4.8845746 3.2762858 0.3814932
H -3.9948640 3.2218941 1.9251249
C -3.5609986 0.4930313 1.9377090
H -2.9594865 1.0087116 2.6932064
H -3.0384679 -0.4229672 1.6502961
H -4.5217357 0.2191777 2.3862883
H -2.5492455 5.9978027 0.1508458
H -3.8059500 4.9693812 0.7859591
C -3.3336427 4.6262882 -1.3027575
H -2.4621426 4.7576727 -1.9574801
C -4.4944512 5.4946160 -1.7948091
H -3.6102216 3.5671766 -1.3755448
H -4.2209020 6.5563346 -1.7127402
H -5.3618557 5.3512937 -1.1333558
C -4.9078970 5.1877013 -3.2380762
H -4.0447300 5.3375460 -3.9020202
C -6.0805310 6.0425294 -3.7299258
H -5.1753064 4.1241002 -3.3189883
H -5.8129307 7.1058884 -3.6496802
H -6.9429296 5.8922736 -3.0644731
C -6.4950239 5.7327243 -5.1720532
H -5.6329402 5.8827119 -5.8379988
C -7.6683427 6.5870682 -5.6647927
H -6.7627340 4.6691212 -5.2524776
H -7.3998337 7.6491779 -5.5828444
H -8.5290242 6.4351509 -4.9990634
C -8.0734489 6.2700912 -7.1076970
H -7.2380160 6.4433888 -7.7962488
H -8.9130041 6.8929699 -7.4349495
H -8.3742055 5.2205746 -7.2086760

3d-H_vac
E(TPSS-D3/def2-TZVP) = -911.5341901688 (conv)
Lowest Freq. = 15.15 cm^-1

60
3d-H_vac (017-H/c1/tpss-d3.def2-TZVP)
C -1.7470828 0.6873886 -0.0252483
C -0.5145372 1.2197134 -0.1967603
N -2.5552001 1.6483889 0.5670838
N -0.5594956 2.5316369 0.2505073
C -1.8226243 2.7884654 0.7149221
N -2.2516978 3.9704459 1.2481639
C -3.9216524 1.2404096 1.1153492
C 0.6192267 3.4865529 0.2383729
C -3.1552191 4.9145367 0.5107542
H -2.1116595 -0.2971250 -0.2606021
H 0.3766753 0.7763911 -0.6025303
C 1.7950834 2.7940085 -0.4623110
H 1.5521184 2.5256067 -1.4944917
H 2.1297622 1.9044075 0.0791842
H 2.6298967 3.4981777 -0.4878024
C 0.2540709 4.7530025 -0.5498454
H 1.1390412 5.3923140 -0.6068000
H -0.5426603 5.3304477 -0.0791825
H -0.0500965 4.4984573 -1.5688017
C 1.0259808 3.7982028 1.6877080
H 0.2728910 4.3730936 2.2359343
H 1.9390163 4.3995841 1.6779664
H 1.2252589 2.8763757 2.2409048
C -4.7448871 0.6914491 -0.0578113
H -4.8908914 1.4546304 -0.8275729
H -5.7264821 0.3878680 0.3156552
H -4.2796072 -0.1845372 -0.5175501
C -4.6715859 2.3975215 1.7739573
H -5.5895001 1.9792554 2.1959842
H -4.9638133 3.1596476 1.0505346
H -4.1001143 2.8571784 2.5808756
C -3.6552920 0.1499119 2.1672282
H -3.0442612 0.5420225 2.9854636
H -3.1517293 -0.7201324 1.7380369
H -4.6116047 -0.1829335 2.5792964
H -2.6426805 5.8825849 0.4864721
H -4.0689502 5.0480067 1.0973915
C -3.4855891 4.4772393 -0.9108356
H -2.5581864 4.3514418 -1.4837454
C -4.3988171 5.4880316 -1.6150997
H -3.9792206 3.4979282 -0.8985600
H -3.9024310 6.4670695 -1.6496606
H -5.3142649 5.6246196 -1.0236427
C -4.7711539 5.0515651 -3.0365170
H -3.8538221 4.9121381 -3.6257469
C -5.6874752 6.0508610 -3.7504187
H -5.2649310 4.0699363 -2.9957954
H -5.1918595 7.0308382 -3.7922725
H -6.6013219 6.1924066 -3.1566306
C -6.0662041 5.6116970 -5.1687435
H -5.1514813 5.4709130 -5.7622074
C -6.9852620 6.6085440 -5.8839977
H -6.5595328 4.6299402 -5.1254671
H -6.4909352 7.5885223 -5.9246420
H -7.8977621 6.7476231 -5.2887747
C -7.3582025 6.1612981 -7.3004112
H -6.4641059 6.0448569 -7.9236559
H -8.0139997 6.8897084 -7.7875856
H -7.8807583 5.1978827 -7.2831927
H -1.5132856 4.4538838 1.7427501

3d-CO2_solv
E(TPSS-D3/def2-TZVP) = -1099.843818810 (conv)
Lowest Freq. = 13.68 cm^-1
62
3d-CO2_solv (017-CO2/c1/tpss-d3.def2-TZVP_COSMO_37.5)

C 0.9964606 -3.1585411 1.1080753
C 2.2122534 -2.5969802 0.8902322
N 0.1849028 -2.1952933 1.6777565
N 2.1510436 -1.2837400 1.3187098
C 0.9013874 -1.0434628 1.8163725
N 0.4550266 0.1355648 2.3527815
C -1.2166420 -2.5472850 2.1352076
C 3.3910737 -0.4111827 1.3734534
C -0.1849284 1.1832027 1.5323416
H 0.6511565 -4.1572117 0.9020243
H 3.1023994 -3.0285696 0.4674950
C 4.1945675 -0.6633989 0.0887042
H 3.5912076 -0.4490623 -0.7987373
H 4.5736797 -1.6862370 0.0258314
H 5.0573634 0.0078427 0.0921109
C 3.0555781 1.0813970 1.4476976
H 4.0017859 1.6231223 1.3598685
H 2.5898562 1.3627410 2.3916762
H 2.4150336 1.3910514 0.6182900
C 4.1804836 -0.8465209 2.6167405
H 3.5716280 -0.7063336 3.5140243
H 5.0875997 -0.2398053 2.6951500
H 4.4714134 -1.8991660 2.5424838
C -1.9689766 -3.0972546 0.9142701
H -2.0407996 -2.3372787 0.1302135
H -2.9805447 -3.3742423 1.2235259
H -1.4858554 -3.9861541 0.5004446
C -1.9844147 -1.3532368 2.7044613
H -2.9801539 -1.7234629 2.9670175
H -2.1093213 -0.5532578 1.9727932
H -1.5188418 -0.9571960 3.6072197
C -1.0614956 -3.6171806 3.2277775
H -0.4822290 -3.2167502 4.0645696
H -0.5649570 -4.5137527 2.8457567
H -2.0545306 -3.9018449 3.5869687
H 0.4280113 2.0905619 1.5871850
H -1.1528274 1.4224855 1.9871858
C -0.3749419 0.7662069 0.0766190
H 0.5924520 0.5013993 -0.3698211
C -1.0237950 1.8821498 -0.7485500
H -0.9992869 -0.1347617 0.0214573
H -0.3995575 2.7844304 -0.6920835
H -1.9947622 2.1432382 -0.3059594
C -1.2208714 1.4901846 -2.2165906
H -0.2475101 1.2254834 -2.6536897
C -1.8675036 2.5984445 -3.0541021
H -1.8426558 0.5850610 -2.2693899
H -1.2468997 3.5042086 -2.9965662
H -2.8419131 2.8605672 -2.6174988
C -2.0597597 2.2101548 -4.5239841
H -1.0848857 1.9479073 -4.9601590
C -2.7064635 3.3174047 -5.3641779
H -2.6795797 1.3035582 -4.5816863
H -2.0866336 4.2226265 -5.3044794
H -3.6804155 3.5779337 -4.9275133
C -2.8927649 2.9196572 -6.8322997
H -1.9285800 2.6818324 -7.2977969
H -3.3559526 3.7273428 -7.4100686
H -3.5327815 2.0331835 -6.9185103
C 0.6547367 0.3331820 3.7704792
O 1.1794142 -0.6435069 4.3712537
O 0.2794946 1.4433617 4.2178274

3x_solv
E(TPSS-D3/def2-TZVP) = -399.7351856581 (conv)
Lowest Freq. = 44.23 cm^-1
20
3x_solv (001/c1/tpss-d3.def2-TZVP_COSMO_37.5)

C -2.0484540 0.8333552 0.0008613
C -0.7636576 1.2472439 -0.0789202
N -2.8581494 1.9640281 0.1826153
N -0.7632582 2.6335372 0.0384395
C -2.0609213 3.1151677 0.1772700
N -2.2976508 4.3905068 0.2725700
C -4.3134560 1.8960757 0.0544385
H -4.6373559 2.1924801 -0.9487974
H -4.7997706 2.5267182 0.7968049
H -4.6096390 0.8601179 0.2287158
C 0.3945534 3.5080702 0.0014699
H 0.3678621 4.1463747 -0.8881955
H 1.2924579 2.8887482 -0.0187759
H 0.4053159 4.1491776 0.8879213
C -3.6430196 4.8861881 0.5411139
H -3.5970714 5.9793478 0.5886739
H -4.0431406 4.5382813 1.5069849
H -4.3786887 4.6281167 -0.2356214
H 0.1527273 0.6882938 -0.1848359
H -2.4755636 -0.1565292 -0.0343827

3x_vac
E(TPSS-D3/def2-TZVP) = -399.7236019258 (conv)
Lowest Freq. = 34.73 cm^-1
20
3x_vac (001/c1/tpss-d3.def2-TZVP)
C -2.0460461 0.8187191 -0.0133253
C -0.7660778 1.2423933 -0.0972677
N -2.8620758 1.9398250 0.2045625
N -0.7672627 2.6231734 0.0502327
C -2.0693543 3.1048720 0.2009799
N -2.2970944 4.3690753 0.3061148
C -4.3065477 1.8787490 0.0326621
H -4.5991793 2.0591774 -1.0098056
H -4.8003224 2.6064539 0.6738651
H -4.6392306 0.8784012 0.3219748
C 0.3702924 3.5180967 -0.0068776
H 0.3695084 4.0928770 -0.9401740
H 1.2849892 2.9252187 0.0614969
H 0.3143810 4.2252667 0.8249398
C -3.6184342 4.9006673 0.5769067
H -3.5380273 5.9901708 0.6437821
H -4.0360816 4.5495170 1.5358733
H -4.3578827 4.6815923 -0.2105910
H 0.1502524 0.6861276 -0.2140217
H -2.4626864 -0.1750736 -0.0529777

3x-H_vac
E(TPSS-D3/def2-TZVP) = -400.1393645523 (conv)
Lowest Freq. = 55.82 cm^-1
21
3x-H_vac (001-H/c1/tpss-d3.def2-TZVP)
C -2.0332795 0.8231702 0.0779919
C -0.7505068 1.2477012 0.0374471
N -2.8553221 1.9536298 0.0725310
N -0.7772204 2.6424400 0.0288191
C -2.0692183 3.0579450 0.0425197
N -2.4602017 4.3510424 -0.0226341
C -4.3202934 1.9074730 -0.0478097
H -4.6342771 2.4790663 -0.9231894
H -4.7962345 2.2958902 0.8536184
H -4.6032641 0.8642960 -0.1818787
C 0.3907186 3.5275578 0.0096461
H 0.4746938 4.0311190 -0.9577328
H 1.2788070 2.9186248 0.1726030
H 0.3119619 4.2616272 0.8162420
C -3.6450692 4.9073026 0.6627468
H -3.5406392 5.9918078 0.6523882

H -3.6999686 4.5657357 1.7007233
H -4.5628474 4.6491544 0.1328828
H 0.1787380 0.7022001 0.0227102
H -2.4513002 -0.1695466 0.1089053
H -1.7040289 5.0064180 -0.1707680

3x-CO2_solv
E(TPSS-D3/def2-TZVP) = -588.4579978385 (conv)
Lowest Freq. = 69.07 cm^-1
23
3x-CO2_solv (001-CO2/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C 0.1744729 -1.9959597 -0.2297197
C 1.4731268 -1.6400736 -0.0291798
N -0.5749919 -0.8316581 -0.2089065
N 1.5008969 -0.2677846 0.1454537
C 0.2447367 0.2252748 0.0230982
N -0.1269567 1.5314935 0.1382859
C -2.0180735 -0.7349731 -0.4413996
H -2.2243429 0.2101532 -0.9442510
H -2.5596397 -0.7819050 0.5057407
H -2.3152087 -1.5658394 -1.0802480
C 2.6920579 0.5396422 0.4069853
H 3.1215770 0.8754786 -0.5378200
H 3.4018341 -0.0718599 0.9639385
H 2.3944363 1.4055107 0.9993830
C -1.1292225 1.9294893 1.1403697
H -2.0937852 2.1592406 0.6774422
H -0.7662506 2.8187055 1.6592722
H -1.2521887 1.1178658 1.8606804
H 2.3713273 -2.2346375 0.0107457
H -0.2801932 -2.9602023 -0.3887812
C 0.3758916 2.5115593 -0.8280503
O -0.0193014 3.6834084 -0.6348470
O 1.1261045 2.0411199 -1.7186352

3y_solv
E(TPSS-D3/def2-TZVP) = -557.0923718285 (conv)
Lowest Freq. = 24.01 cm^-1
32
3y_solv (026/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -2.0214389 0.7121319 -0.4904039
C -0.7632434 1.1822331 -0.6333571
N -2.8609836 1.7945614 -0.1729232
N -0.7925676 2.5538447 -0.4023606
C -2.0840503 2.9593886 -0.0639483
N -2.3404912 4.1947487 0.2485010
C -4.1885542 1.6003509 0.4535315
C 0.3552324 3.4679302 -0.3485403
C -3.7006494 4.6833753 0.4149408
H -3.6574780 5.7726150 0.5243355
H -4.2075478 4.2941967 1.3129203
H -4.3486357 4.4704987 -0.4513663
H -2.4070871 -0.2848017 -0.6224294
H 0.1399159 0.6698688 -0.9223590
C 1.3959871 3.1035757 -1.4070169
H 0.9458254 3.0617045 -2.4038038
H 1.8665439 2.1374999 -1.1934507
H 2.1836451 3.8630398 -1.4123896
C 0.9455052 3.5005149 1.0665093
H 0.1711197 3.7723039 1.7899614
H 1.7532777 4.2379350 1.1237539
H 1.3524996 2.5187245 1.3346225
C -4.9487552 0.4630689 -0.2303675
H -4.9958913 0.6177847 -1.3126674

H -5.9697332 0.4360840 0.1617054
H -4.4905752 -0.5110387 -0.0311689
C -4.0382965 1.3723442 1.9618906
H -3.4988744 2.2046920 2.4253764
H -3.4836233 0.4476047 2.1557760
H -5.0244939 1.2924040 2.4310135
H -0.0703561 4.4510542 -0.5729935
H -4.7463657 2.5198800 0.2855834

3y_vac
E(TPSS-D3/def2-TZVP) = -557.0825317304 (conv)
Lowest Freq. = 34.79 cm^-1
32
3y_vac (026/c1/tpss-d3.def2-TZVP)
C -2.0477808 0.7093942 -0.5794291
C -0.7862007 1.1748192 -0.7000197
N -2.8849222 1.7888237 -0.2406559
N -0.8035458 2.5377503 -0.4304429
C -2.0952349 2.9473548 -0.0875215
N -2.3328054 4.1652672 0.2689609
C -4.1786049 1.5966705 0.4437818
C 0.3347927 3.4570539 -0.3446098
C -3.6728055 4.6929715 0.4211915
H -3.5975261 5.7792748 0.5350610
H -4.2018167 4.3170109 1.3136213
H -4.3169084 4.5016412 -0.4541072
H -2.4387909 -0.2773064 -0.7603779
H 0.1108346 0.6654106 -1.0111216
C 1.4149078 3.0887921 -1.3608792
H 1.0011248 3.0241959 -2.3719629
H 1.8917853 2.1325883 -1.1161106
H 2.1953819 3.8556549 -1.3541611
C 0.8706612 3.5138257 1.0911393
H 0.0650958 3.8005607 1.7721865
H 1.6744762 4.2540372 1.1697217
H 1.2673411 2.5379417 1.3945437
C -4.9594970 0.4424749 -0.1863685
H -5.0463372 0.5717419 -1.2693747
H -5.9659681 0.4133517 0.2417795
H -4.4878506 -0.5247013 0.0167906
C -3.9652075 1.3986542 1.9495105
H -3.4103766 2.2431646 2.3695152
H -3.3943990 0.4826304 2.1370060
H -4.9280182 1.3217491 2.4663529
H -0.0933840 4.4350424 -0.5896808
H -4.7485611 2.5122779 0.2845361

3y-H_vac
E(TPSS-D3/def2-TZVP) = -557.5038872916 (conv)
Lowest Freq. = 45.24 cm^-1
33
3y-H_vac (026-H/c1/tpss-d3.def2-TZVP)
C -2.0286733 0.7287377 -0.5951306
C -0.7756744 1.2137965 -0.7507826
N -2.8234378 1.7525104 -0.0743832
N -0.7921740 2.5475918 -0.3475583
C -2.0449403 2.8542007 0.0790196
N -2.3992653 4.0491249 0.6148386
C -4.2138963 1.5735069 0.4551120
C 0.3657324 3.4841225 -0.3327115
C -3.6936255 4.7217476 0.3966907
H -3.5400939 5.7854629 0.5788655
H -4.4487932 4.3607648 1.0990067
H -4.0422676 4.5882039 -0.6315709
H -2.4333865 -0.2428698 -0.8169146
H 0.1152365 0.7453556 -1.1315270
C 1.3482641 3.1403827 -1.4502440
H 0.8491414 3.0845012 -2.4213038

H 1.8627975 2.1950335 -1.2536312
H 2.1087518 3.9236357 -1.4983538
C 1.0235824 3.4868730 1.0513343
H 0.3089507 3.7301527 1.8443423
H 1.8269496 4.2280295 1.0748188
H 1.4535326 2.5047562 1.2694002
C -4.8749907 0.3537883 -0.1804475
H -4.8439221 0.3981442 -1.2728140
H -5.9230885 0.3340363 0.1281743
H -4.4157519 -0.5794782 0.1592865
C -4.1689543 1.4914891 1.9827744
H -3.6910754 2.3732539 2.4194801
H -3.6165653 0.6021711 2.3009431
H -5.1879458 1.4230504 2.3734115
H -0.0640677 4.4703638 -0.5481345
H -4.7686948 2.4602572 0.1433312
H -1.6191395 4.6705042 0.7793123

3y-CO2_solv
E(TPSS-D3/def2-TZVP) = -745.8175555657 (conv)
Lowest Freq. = 28.50 cm^-1
35
3y-CO2_solv (026-CO2/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -1.8532691 0.6550584 0.2072803
C -0.6278061 1.1383268 -0.1441921
N -2.6832032 1.7441459 0.3951950
N -0.7236141 2.5168859 -0.1668104
C -1.9823314 2.8824132 0.1754596
N -2.4627992 4.1632073 0.2609120
C -4.0981749 1.7063412 0.8426950
C 0.3790961 3.4717742 -0.4423962
C -3.0526253 4.8002404 -0.9221748
H -3.3545444 5.7994291 -0.6071339
H -3.9294452 4.2465196 -1.2766423
H -2.3241259 4.8767248 -1.7373296
H -2.1952756 -0.3592891 0.3325598
H 0.2872020 0.6197484 -0.3794023
C 0.9451259 3.2280555 -1.8408790
H 0.1595057 3.2952732 -2.5990349
H 1.4186607 2.2431908 -1.9087280
H 1.7036307 3.9861089 -2.0547766
C 1.4304001 3.3724656 0.6638609
H 0.9713198 3.5417010 1.6413816
H 2.1988370 4.1324628 0.4962313
H 1.9123132 2.3892313 0.6584826
C -4.9400061 0.9050815 -0.1496750
H -4.8506288 1.3146518 -1.1600202
H -5.9891348 0.9516068 0.1550920
H -4.6360274 -0.1466019 -0.1661637
C -4.1685449 1.1676472 2.2722731
H -3.5403746 1.7672494 2.9362494
H -3.8410906 0.1235645 2.3134412
H -5.2034966 1.2170279 2.6225212
H -0.0998285 4.4528086 -0.4009866
H -4.4096614 2.7534177 0.8337208
C -2.3540838 4.8263660 1.5546730
O -2.7983296 5.9958707 1.6155694
O -1.8185321 4.1156828 2.4447544

4a_solv
E(TPSS-D3/def2-TZVP) = -635.7715586481 (conv)
Lowest Freq. = 35.04 cm^-1
38
4a_solv (018/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -2.1107558 0.8552184 -0.6329350
C -0.8447663 1.3330759 -0.7349489
N -2.9409195 1.9091365 -0.1559348
N -0.8511645 2.6736944 -0.3035961

C -2.1513882 3.0563857 0.0187198
N -2.4495262 4.2770459 0.3526904
C -4.1150800 1.6666591 0.7223526
C 0.2115037 3.6851469 -0.4304916
C -3.8290556 4.7389611 0.3546535
H -3.8318625 5.8114001 0.1229528
H -4.3277012 4.6311624 1.3320128
H -4.4589328 4.2353965 -0.3970889
C -2.6361446 -0.4822865 -1.0360902
C 0.3801330 0.6235639 -1.2080292
C 1.5007315 3.2843537 0.2925726
H 2.0401923 2.4901210 -0.2301874
H 1.2840768 2.9489534 1.3116685
H 2.1620370 4.1554181 0.3486033
C 0.4434898 4.0782905 -1.8951415
H 1.1509797 4.9129494 -1.9465107
H -0.4979813 4.3933284 -2.3559052
H 0.8563937 3.2485896 -2.4774992
C -5.3133519 1.0988403 -0.0425784
H -5.5357928 1.7162907 -0.9183862
H -6.1896616 1.0998110 0.6140354
H -5.1437053 0.0715660 -0.3738454
C -3.7297387 0.8276988 1.9480550
H -2.8878024 1.2880237 2.4750801
H -3.4507591 -0.1935600 1.6736039
H -4.5804673 0.7744369 2.6355548
H -1.8147879 -1.0957108 -1.4141527
H -3.3853779 -0.3948808 -1.8325297
H -3.1003920 -1.0298578 -0.2081523
H 0.1031618 -0.3574365 -1.6000853
H 1.0973686 0.4670963 -0.3940362
H 0.8977110 1.1682171 -2.0046923
H -4.3981154 2.6514494 1.0860152
H -0.2181382 4.5484210 0.0844065

4a_vac
E(TPSS-D3/def2-TZVP) = -635.7621380744 (conv)
Lowest Freq. = 35.65 cm^-1
38
4a_vac (018/c1/tpss-d3.def2-TZVP)
C -2.1143821 0.8420315 -0.6406537
C -0.8495189 1.3221212 -0.7412794
N -2.9516153 1.8971953 -0.1802655
N -0.8558686 2.6616686 -0.3180206
C -2.1621325 3.0529301 -0.0076226
N -2.4445430 4.2702982 0.3114463
C -4.1164314 1.6641979 0.7048452
C 0.1989791 3.6791213 -0.4279001
C -3.8036232 4.7640242 0.3676108
H -3.7861327 5.8379405 0.1477041
H -4.2628207 4.6594676 1.3654434
H -4.4779292 4.2861858 -0.3638354
C -2.6352647 -0.4966456 -1.0418225
C 0.3766389 0.6149477 -1.2123678
C 1.4848445 3.2828651 0.3034290
H 2.0376033 2.4965311 -0.2186960
H 1.2610546 2.9387915 1.3177254
H 2.1415382 4.1564972 0.3743597
C 0.4400083 4.0893089 -1.8865040
H 1.1415219 4.9298564 -1.9273245
H -0.5008886 4.4030845 -2.3474591
H 0.8625017 3.2695797 -2.4770506
C -5.3138073 1.0703732 -0.0434348
H -5.5386554 1.6640393 -0.9343352
H -6.1922256 1.0804121 0.6107487
H -5.1396157 0.0361278 -0.3502629
C -3.7228760 0.8544080 1.9481193
H -2.8887548 1.3373901 2.4660158

H -3.4238050 -0.1660718 1.6914697
H -4.5714839 0.7954850 2.6383368
H -1.8133344 -1.1102361 -1.4188888
H -3.3851646 -0.4140467 -1.8387103
H -3.0976948 -1.0468413 -0.2133349
H 0.1055205 -0.3687277 -1.6020133
H 1.0963887 0.4639248 -0.3991695
H 0.8914787 1.1597053 -2.0113888
H -4.4065712 2.6559727 1.0454804
H -0.2485288 4.5330564 0.0897659

4a-H_vac
E(TPSS-D3/def2-TZVP) = -636.1902183431 (conv)
Lowest Freq. = -9.51 cm^-1
39
4a-H_vac (018-H/c1/tpss-d3.def2-TZVP)
C -2.0346413 0.7711416 -0.4768038
C -0.8211677 1.3491437 -0.7502470
N -2.8100635 1.7322028 0.1819005
N -0.8823919 2.6708817 -0.2863168
C -2.0975344 2.8785486 0.2797335
N -2.5660375 4.0215042 0.8845259
C -4.1420365 1.5639611 0.8420643
C 0.1287083 3.7552206 -0.4625958
C -3.5115838 4.8904933 0.1422087
H -3.0361284 5.3968975 -0.7064383
H -3.9065782 5.6317425 0.8380817
H -4.3398426 4.2832395 -0.2270934
C -2.5063385 -0.6015626 -0.8217964
C 0.3792698 0.7293726 -1.3838844
C 1.4665293 3.4024053 0.1897116
H 2.0051147 2.6374649 -0.3727138
H 1.3276227 3.0552304 1.2174589
H 2.0914907 4.2993809 0.2119587
C 0.2472141 4.1604034 -1.9346422
H 0.8795739 5.0497400 -2.0056427
H -0.7326945 4.3988190 -2.3573099
H 0.7073840 3.3757989 -2.5392707
C -5.2348179 1.2139183 -0.1686260
H -5.2239729 1.8988682 -1.0216887
H -6.2072650 1.2969003 0.3243890
H -5.1370880 0.1910765 -0.5386712
C -4.0510630 0.5865586 2.0163745
H -3.2442443 0.8684945 2.6981572
H -3.8951003 -0.4437270 1.6893026
H -4.9939553 0.6195075 2.5695038
H -1.6740711 -1.1785171 -1.2275008
H -3.2949281 -0.5743752 -1.5801095
H -2.8881789 -1.1408975 0.0481678
H 0.1043160 -0.2385706 -1.8056335
H 1.1767943 0.5598153 -0.6533738
H 0.7835982 1.3388134 -2.1954771
H -4.3391904 2.5562977 1.2523235
H -0.2999733 4.6018978 0.0803510
H -1.8459268 4.5446600 1.3708578

4a-CO2_solv
E(TPSS-D3/def2-TZVP) = -824.5009701921 (conv)
Lowest Freq. = 33.44 cm^-1
41
4a-CO2_solv (018-CO2/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -2.0263526 0.7865947 -0.5181316
C -0.8626660 1.3905057 -0.9321178
N -2.7685059 1.7547663 0.1569108
N -0.9173259 2.7154996 -0.5016225
C -2.0760687 2.9176612 0.1679411
N -2.4869280 4.0982397 0.7374243
C -4.0665305 1.6125475 0.8711081

C 0.1140750 3.7822261 -0.6169161
C -3.2612998 5.0538490 -0.0623848
H -2.6868659 5.4076888 -0.9265373
H -3.4819414 5.8930981 0.5976185
H -4.1977219 4.6071755 -0.4157556
C -2.4791726 -0.6136880 -0.7607415
C 0.2503984 0.8026898 -1.7324259
C 1.3103494 3.4742917 0.2867155
H 1.8762470 2.6080787 -0.0671775
H 0.9703012 3.2895245 1.3089257
H 1.9804842 4.3391739 0.2878373
C 0.4904814 4.0534069 -2.0735153
H 1.0884590 4.9686520 -2.1096345
H -0.4025706 4.1994691 -2.6882169
H 1.0873776 3.2444952 -2.5010354
C -5.1736882 1.1113741 -0.0562937
H -5.2087317 1.6998259 -0.9778740
H -6.1313752 1.2213925 0.4605599
H -5.0489638 0.0568446 -0.3128924
C -3.8930187 0.7753831 2.1404509
H -3.0881820 1.1878637 2.7543670
H -3.6717859 -0.2707446 1.9115458
H -4.8254515 0.8073872 2.7120795
H -1.6328235 -1.2109768 -1.1055470
H -3.2558286 -0.6566746 -1.5316019
H -2.8726013 -1.0798457 0.1456438
H 0.1517460 -0.2846285 -1.7410166
H 1.2296186 1.0480730 -1.3145708
H 0.2257576 1.1496621 -2.7708792
H -4.2980584 2.6375949 1.1689834
H -0.3950829 4.6624380 -0.2181301
C -2.1140406 4.3412196 2.1230540
O -2.4962174 5.4279274 2.6174468
O -1.4470252 3.4085827 2.6431183

4b_solv
E(TPSS-D3/def2-TZVP) = -753.7815152942 (conv)
Lowest Freq. = 29.57 cm^-1
47
4b_solv (019/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -2.0649225 0.7252815 -0.5927479
C -0.8163831 1.2461094 -0.7123313
N -2.9458316 1.7788186 -0.2331044
N -0.8933544 2.6165623 -0.4141073
C -2.2128584 2.9741402 -0.1184591
N -2.5222088 4.1869979 0.2190184
C -4.1360064 1.5751026 0.6236332
C 0.1272974 3.6576006 -0.6115961
C -3.7569680 4.9317177 -0.0504073
C -3.2837438 6.3381724 -0.4863441
C -4.6070502 5.1130895 1.2258101
C -4.6061859 4.3573801 -1.2004954
C -2.5208727 -0.6693144 -0.8662552
C 0.4494130 0.5487654 -1.0862261
C 1.3968925 3.4087902 0.2078789
H 1.9923406 2.5816852 -0.1887691
H 1.1458279 3.1900351 1.2505868
H 2.0198697 4.3093592 0.1843881
C 0.4096923 3.8980222 -2.0999384
H 1.0753861 4.7605917 -2.2132639
H -0.5232300 4.1093624 -2.6321510
H 0.8917920 3.0358648 -2.5713377
C -5.2649111 0.8139582 -0.0765338
H -5.4549113 1.2240130 -1.0730756
H -6.1796149 0.9102280 0.5176547
H -5.0426662 -0.2508891 -0.1769145
C -3.7453602 0.9493400 1.9688189
H -2.9736263 1.5518271 2.4583004

H -3.3647026 -0.0687258 1.8428203
H -4.6209847 0.9070836 2.6250855
H -1.6683876 -1.2740064 -1.1848799
H -3.2713706 -0.6975747 -1.6652659
H -2.9583505 -1.1565962 0.0130144
H 0.2255392 -0.4773941 -1.3858354
H 1.1504014 0.5051211 -0.2447187
H 0.9653981 1.0355425 -1.9204151
H -4.4864225 2.5855728 0.8234174
H -0.3749971 4.5456505 -0.2164265
H -3.9815211 4.2127045 -2.0891188
H -5.4091096 5.0590111 -1.4542850
H -5.0682495 3.4005323 -0.9497332
H -2.6895160 6.2622421 -1.4033281
H -2.6530129 6.7743649 0.2953778
H -4.1355090 7.0051883 -0.6691135
H -5.4289956 5.8155922 1.0429000
H -3.9798724 5.5139612 2.0295293
H -5.0430029 4.1716386 1.5754239

4b_vac
E(TPSS-D3/def2-TZVP) = -753.7738914943 (conv)
Lowest Freq. = 29.75 cm^-1
47
4b_vac (019/c1/tpss-d3.def2-TZVP)
C -2.0642923 0.7160747 -0.6013340
C -0.8155573 1.2353364 -0.7073015
N -2.9569750 1.7744470 -0.2810920
N -0.8925663 2.6081833 -0.4321384
C -2.2237599 2.9793159 -0.1844688
N -2.5243681 4.2028955 0.0775601
C -4.1298520 1.5795598 0.5969519
C 0.1360843 3.6448249 -0.5865103
C -3.7739039 4.9403095 -0.0923547
C -3.3342559 6.3532381 -0.5417757
C -4.5271448 5.1050447 1.2459543
C -4.7006846 4.3768628 -1.1882689
C -2.5174218 -0.6783523 -0.8747139
C 0.4527735 0.5349902 -1.0637241
C 1.3898414 3.3699986 0.2491684
H 1.9968058 2.5570082 -0.1598936
H 1.1180097 3.1197038 1.2790333
H 2.0135956 4.2701177 0.2681998
C 0.4461661 3.9202967 -2.0633828
H 1.1212878 4.7789071 -2.1490379
H -0.4763499 4.1525225 -2.6035817
H 0.9273252 3.0647759 -2.5488083
C -5.2643300 0.8013925 -0.0763344
H -5.4704356 1.2011622 -1.0734343
H -6.1729728 0.8937400 0.5282593
H -5.0361854 -0.2629067 -0.1710255
C -3.7187935 0.9808890 1.9488840
H -2.9496520 1.6013384 2.4183414
H -3.3237978 -0.0333141 1.8360960
H -4.5846921 0.9363606 2.6183013
H -1.6635559 -1.2855293 -1.1853960
H -3.2620934 -0.7090765 -1.6796543
H -2.9613891 -1.1670185 0.0015841
H 0.2316318 -0.4896457 -1.3707174
H 1.1428700 0.4856885 -0.2133567
H 0.9814907 1.0236038 -1.8893641
H -4.4864136 2.5901284 0.7843911
H -0.3685028 4.5264344 -0.1784931
H -4.1369876 4.2392179 -2.1171418
H -5.5176979 5.0810166 -1.3831063
H -5.1473814 3.4178593 -0.9183305
H -2.8055859 6.2914743 -1.4985543
H -2.6504714 6.7785042 0.1990885

H -4.1971567 7.0205376 -0.6565429
H -5.3580088 5.8115414 1.1333414
H -3.8397220 5.4919141 2.0045063
H -4.9397841 4.1611468 1.6166569

4b-H_vac
E(TPSS-D3/def2-TZVP) = -754.2114144379 (conv)
Lowest Freq. = 25.35 cm^-1
48
4b-H_vac (019-H/c1/tpss-d3.def2-TZVP)
C -2.0460139 0.6954435 -0.4752917
C -0.8690974 1.3230580 -0.8012702
N -2.8729125 1.6522532 0.1144091
N -1.0051258 2.6638240 -0.4290193
C -2.2317930 2.8490219 0.1312045
N -2.7464923 3.9914316 0.6863877
C -4.1631063 1.4326099 0.8368360
C -0.0332813 3.7768250 -0.6273882
C -3.6507180 4.9595040 -0.0585328
C -2.8246168 6.1754865 -0.5021023
C -4.7443555 5.3946000 0.9235462
C -4.2564493 4.2636100 -1.2771195
C -2.4304663 -0.7282150 -0.7030204
C 0.3570369 0.7285004 -1.4099678
C 1.2849314 3.5201188 0.1053808
H 1.8787906 2.7429772 -0.3798843
H 1.1104404 3.2338127 1.1464839
H 1.8743279 4.4412323 0.0972518
C 0.1442013 4.1029246 -2.1125342
H 0.7152213 5.0312120 -2.2031838
H -0.8223125 4.2437179 -2.6040496
H 0.6944498 3.3222719 -2.6421469
C -5.2168783 0.7489823 -0.0352326
H -5.2800171 1.2070841 -1.0260583
H -6.1897444 0.8563483 0.4524975
H -5.0242140 -0.3189975 -0.1540301
C -3.9058862 0.7089584 2.1609429
H -3.1785457 1.2548440 2.7679633
H -3.5413685 -0.3100290 2.0064927
H -4.8439446 0.6480931 2.7199974
H -1.5567044 -1.2911189 -1.0344894
H -3.2007639 -0.8175906 -1.4752739
H -2.8042467 -1.2045255 0.2069418
H 0.1337508 -0.2821505 -1.7550338
H 1.1745261 0.6596414 -0.6853147
H 0.7117865 1.2988602 -2.2713985
H -4.4914921 2.4483435 1.0630188
H -0.5270333 4.6291666 -0.1551820
H -3.4822294 3.8989542 -1.9609963
H -4.8745462 4.9809933 -1.8228308
H -4.8963457 3.4257230 -0.9898100
H -2.0751048 5.8987083 -1.2497370
H -2.3184797 6.6381816 0.3532441
H -3.4786636 6.9315233 -0.9469120
H -5.4059665 6.1284167 0.4535203
H -4.3062468 5.8544937 1.8152321
H -5.3471718 4.5381890 1.2403975
H -2.0980581 4.4768533 1.2989602

4b-CO2_solv
E(TPSS-D3/def2-TZVP) = -942.5152691700 (conv)
Lowest Freq. = 13.66 cm^-1
50
4b-CO2_solv (019-CO2/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C 0.2395872 -2.1441635 -0.2928959
C 1.3495580 -1.5108737 -0.7977168
N -0.5198873 -1.1742427 0.3593694
N 1.2459849 -0.1665377 -0.4443175

C 0.1058872 0.0250051 0.2645115
N -0.3318826 1.2166610 0.7971939
C -1.7459808 -1.3568983 1.1810183
C 2.2424839 0.9203945 -0.6369376
C -1.2258145 2.1462760 0.0047728
C -0.5180260 3.4947474 -0.2024391
C -2.5532598 2.3486640 0.7525408
C -1.5127406 1.5149475 -1.3633602
C -0.1550227 -3.5752232 -0.4382897
C 2.4485990 -2.0890984 -1.6240956
C 3.4740685 0.6837625 0.2407871
H 4.0602636 -0.1739726 -0.1002875
H 3.1674112 0.5239355 1.2773930
H 4.1130141 1.5707973 0.1926618
C 2.5715448 1.1459463 -2.1126074
H 3.1390954 2.0769920 -2.2002957
H 1.6610581 1.2405480 -2.7113809
H 3.1823847 0.3397231 -2.5249895
C -2.8887276 -1.9840309 0.3825710
H -3.0384605 -1.4656859 -0.5689251
H -3.8073025 -1.8963294 0.9701092
H -2.7172523 -3.0441535 0.1831468
C -1.4174975 -2.1017125 2.4772769
H -0.5939253 -1.6033475 2.9945288
H -1.1495001 -3.1455246 2.2912221
H -2.3014930 -2.0889883 3.1220055
H 0.6979178 -4.1476782 -0.8078095
H -0.9748612 -3.6947050 -1.1544879
H -0.4672642 -4.0136902 0.5125796
H 2.3941204 -3.1787102 -1.5836099
H 3.4352248 -1.7887771 -1.2634353
H 2.3628899 -1.7878670 -2.6734981
H -2.0207517 -0.3328558 1.4400619
H 1.7206651 1.8000921 -0.2562768
H -0.5963250 1.3603533 -1.9412437
H -2.1573387 2.1936876 -1.9294880
H -2.0331624 0.5569347 -1.2686538
H 0.3822628 3.3717169 -0.8138025
H -0.2416671 3.9282060 0.7601818
H -1.1907277 4.1823209 -0.7265117
H -3.1770401 3.0601450 0.2006680
H -2.3668558 2.7375865 1.7549238
H -3.1039232 1.4050703 0.8295682
C 0.1459104 1.4866063 2.1495346
O -0.2115754 2.5620417 2.6821214
O 0.8783337 0.5719050 2.6166071

4c_solv
E(TPSS-D3/def2-TZVP) = -596.4531789245 (conv)
Lowest Freq. = 23.76 cm^-1
35
4c_solv (020/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -2.0359505 0.7760781 -0.4905186
C -0.8265705 1.3238643 -0.7856680
N -2.7675980 1.7369284 0.2458473
N -0.7928361 2.6120217 -0.2149467
C -1.9888144 2.8731547 0.4310509
N -2.2420059 3.9944378 1.0613520
C -4.0719533 1.5748628 0.9081333
C 0.2438791 3.6530955 -0.3214808
C -2.5617888 -0.5699850 -0.8635987
C 0.3070903 0.7200654 -1.5454839
C 1.6115481 3.1813265 0.1827015
H 2.0852157 2.4774412 -0.5066772
H 1.5194908 2.7045682 1.1635507
H 2.2725389 4.0487040 0.2807589
C 0.3033569 4.2464908 -1.7345302
H 0.9938841 5.0965314 -1.7476341

H -0.6857604 4.5985425 -2.0432788
H 0.6563210 3.5131416 -2.4662599
C -5.1763644 1.1074915 -0.0463066
H -5.1687375 1.6985525 -0.9670777
H -6.1451799 1.2433926 0.4446279
H -5.0781472 0.0505696 -0.3039568
C -3.9594320 0.6999022 2.1630820
H -3.1956401 1.0966093 2.8389209
H -3.6953943 -0.3302059 1.9049393
H -4.9181156 0.6842611 2.6919458
H -1.7561080 -1.1607858 -1.3052597
H -3.3734231 -0.5103462 -1.5980776
H -2.9395045 -1.1229008 0.0034068
H -0.0139489 -0.2285859 -1.9814180
H 1.1724423 0.5172503 -0.9039850
H 0.6459745 1.3630373 -2.3647851
H -4.3405455 2.5864166 1.2271432
H -0.1219102 4.4277761 0.3577052
H -3.1702828 3.9625456 1.4832678

4c_vac
E(TPSS-D3/def2-TZVP) = -596.4394680917 (conv)
Lowest Freq. = 24.93 cm^-1
35
4c_vac (020/c1/tpss-d3.def2-TZVP)
C -2.0460124 0.7739291 -0.5102919
C -0.8335354 1.3183118 -0.7951208
N -2.7871963 1.7408480 0.2089181
N -0.7984384 2.6061756 -0.2331102
C -2.0022036 2.8817545 0.4068747
N -2.2298312 3.9998225 1.0248357
C -4.0685146 1.5741969 0.8994914
C 0.2365034 3.6465684 -0.3159769
C -2.5744401 -0.5670291 -0.8931751
C 0.3021512 0.7130480 -1.5490407
C 1.5950838 3.1765768 0.2139586
H 2.0862180 2.4738335 -0.4654601
H 1.4826595 2.6991252 1.1918936
H 2.2557449 4.0424399 0.3286641
C 0.3218089 4.2493184 -1.7238230
H 1.0082279 5.1031156 -1.7219339
H -0.6631634 4.5996888 -2.0448926
H 0.6906529 3.5237941 -2.4564268
C -5.1924494 1.0822410 -0.0203316
H -5.2137585 1.6618976 -0.9477192
H -6.1536336 1.2080994 0.4887805
H -5.0866970 0.0238740 -0.2701809
C -3.9220375 0.7208678 2.1671891
H -3.1484596 1.1385927 2.8178559
H -3.6469315 -0.3090694 1.9192902
H -4.8674100 0.6962356 2.7201424
H -1.7718453 -1.1563041 -1.3428005
H -3.3893285 -0.5025384 -1.6250003
H -2.9495321 -1.1312755 -0.0310365
H -0.0123680 -0.2392499 -1.9821012
H 1.1682323 0.5170616 -0.9057392
H 0.6407485 1.3530786 -2.3714834
H -4.3363683 2.5900531 1.2091022
H -0.1514473 4.4148794 0.3599551
H -3.1566994 4.0222885 1.4461830

4c-H_vac
E(TPSS-D3/def2-TZVP) = -596.8606482221 (conv)
Lowest Freq. = 44.40 cm^-1
36
4c-H_vac (020-H/c1/tpss-d3.def2-TZVP)
C -2.0120130 0.7569751 -0.4580572
C -0.8161247 1.3195907 -0.7969730

N -2.7346480 1.7230898 0.2757014
N -0.7903400 2.6126329 -0.2369071
C -1.9642283 2.8266126 0.3932653
N -2.2627838 3.9538749 1.1059109
C -4.0847597 1.5905328 0.8971978
C 0.2973413 3.6348244 -0.2814815
C -2.5172074 -0.6098898 -0.7778242
C 0.2889747 0.7345708 -1.6109230
C 1.6605382 3.0482928 0.0913749
H 2.0915774 2.4579475 -0.7185944
H 1.5942922 2.4317787 0.9918570
H 2.3434250 3.8773915 0.2958730
C 0.2977598 4.3675112 -1.6260130
H 1.0320954 5.1772518 -1.5973459
H -0.6830640 4.7993466 -1.8482087
H 0.5691457 3.6942815 -2.4434902
C -5.1299257 1.0546023 -0.0841350
H -5.0726078 1.5694769 -1.0470075
H -6.1209762 1.2344619 0.3412458
H -5.0305559 -0.0196750 -0.2448907
C -4.0032343 0.7930795 2.2016203
H -3.2766464 1.2321681 2.8913320
H -3.7174600 -0.2447654 2.0115616
H -4.9834247 0.7902225 2.6864003
H -1.6911098 -1.2157997 -1.1535017
H -3.2985876 -0.5932856 -1.5438822
H -2.9158193 -1.1137293 0.1068876
H -0.0748933 -0.1594192 -2.1200177
H 1.1468581 0.4466673 -0.9954278
H 0.6373859 1.4302611 -2.3790494
H -4.3778418 2.6192198 1.1313871
H 0.0270386 4.3369671 0.5128001
H -3.1697774 3.9816571 1.5522828
H -1.9933956 4.8416487 0.6993581

4c-CO2_solv
E(TPSS-D3/def2-TZVP) = -785.1709019118 (conv)
Lowest Freq. = 27.54 cm^-1
38
4c-CO2_solv (020-CO2/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -2.0040368 0.8140848 -0.5035004
C -0.8236122 1.3790747 -0.9153343
N -2.6496295 1.7597538 0.2990714
N -0.7490930 2.6468428 -0.3325256
C -1.8640511 2.8598434 0.4008844
N -2.1355599 3.9909140 1.1207887
C -3.9773512 1.6695038 0.9650589
C 0.3757930 3.6226147 -0.3701380
C -2.5528578 -0.5325494 -0.8360549
C 0.1966478 0.8089957 -1.8419556
C 1.5803087 3.0856655 0.4067078
H 2.0405511 2.2259762 -0.0874013
H 1.2882963 2.7951551 1.4201200
H 2.3319850 3.8777888 0.4759054
C 0.7016476 4.0535456 -1.7993519
H 1.3943023 4.8993660 -1.7544571
H -0.2076231 4.3754235 -2.3124288
H 1.1821234 3.2560577 -2.3711191
C -5.0838002 1.2892965 -0.0200381
H -5.0317879 1.9055923 -0.9221302
H -6.0475324 1.4679501 0.4653252
H -5.0404172 0.2356786 -0.3032824
C -3.9113326 0.7596378 2.1937524
H -3.1226732 1.0861132 2.8779844
H -3.7236960 -0.2806740 1.9138821
H -4.8692079 0.8041812 2.7202128
H -1.7520804 -1.1574138 -1.2367125
H -3.3431132 -0.4751764 -1.5918310

H -2.9600325 -1.0336357 0.0456098
H 0.0052385 -0.2580900 -1.9720992
H 1.2135814 0.9241050 -1.4596654
H 0.1481957 1.2801242 -2.8292834
H -4.1651806 2.6932103 1.2977158
H -0.0236748 4.4855198 0.1623981
H -2.4752182 3.8717382 2.0685384
C -2.5204278 5.2549313 0.4703147
O -2.9633768 6.1161173 1.2650141
O -2.3366063 5.2960029 -0.7664247

4d_solv
E(TPSS-D3/def2-TZVP) = -439.1022225384 (conv)
Lowest Freq. = 61.04 cm^-1
23
4d_solv (021/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -0.4695966 -0.8829952 -0.2218156
C 0.7877949 -0.4041095 -0.4192992
N -1.2135786 0.1380152 0.4011503
N 0.8136696 0.9108666 0.0910762
C -0.4196589 1.2440950 0.6193392
N -0.8195955 2.3410924 1.2147852
C -2.5890594 0.0567172 0.8614457
C 1.9505277 1.8134856 0.1339465
C -1.0758458 -2.1986328 -0.5687804
C 1.9820792 -1.0326948 -1.0494271
H -1.4624995 -2.7148874 0.3189209
H -0.3236988 -2.8410181 -1.0322920
H -1.9083098 -2.0901725 -1.2759379
H 1.7377971 -2.0483465 -1.3690482
H 2.8274747 -1.0926802 -0.3521123
H 2.3201337 -0.4738777 -1.9316468
H -0.0538416 3.0171048 1.2358135
H -2.6406874 -0.2393306 1.9162045
H -3.1291308 -0.6730492 0.2564708
H -3.0528820 1.0389336 0.7486840
H 2.7925686 1.3483392 -0.3777305
H 2.2377787 2.0273238 1.1701248
H 1.7085608 2.7558207 -0.3698716

4d_vac
E(TPSS-D3/def2-TZVP) = -439.0875561228 (conv)
Lowest Freq. = 35.58 cm^-1
23
4d_vac (021/c1/tpss-d3.def2-TZVP)
C -2.1349715 0.8362841 -0.4991784
C -0.8797393 1.3235571 -0.6801827
N -2.8853722 1.8531985 0.1285129
N -0.8546887 2.6311385 -0.1696551
C -2.0956856 2.9784762 0.3458804
N -2.3625288 4.1233866 0.8917599
C -4.2718603 1.7991297 0.5350572
C 0.2791047 3.5331244 -0.1284561
C -2.7255821 -0.4830827 -0.8530518
C 0.3276625 0.7037271 -1.2926656
H -1.9679580 -1.1107640 -1.3281201
H -3.5644085 -0.3856504 -1.5557677
H -3.0961047 -1.0207707 0.0303768
H 0.1023615 -0.3136425 -1.6206441
H 1.1631674 0.6510040 -0.5825355
H 0.6773570 1.2688228 -2.1665596
H -3.3338447 4.1690750 1.1979884
H -4.6891750 0.8302196 0.2587208
H -4.8527557 2.5872762 0.0395696
H -4.3655348 1.9272614 1.6210940
H 1.0786956 3.1373047 0.5088251
H -0.0864630 4.4720424 0.2912145
H 0.6763842 3.7093120 -1.1340728

4d-H_vac
E(TPSS-D3/def2-TZVP) = -439.5043025530 (conv)
Lowest Freq. = 54.09 cm^-1
24
4d-H_vac (021-H/c1/tpss-d3.def2-TZVP)
C -2.1314795 0.8474894 -0.5182669
C -0.8732603 1.3310297 -0.7104048
N -2.8612568 1.8552192 0.1528874
N -0.8444551 2.6330727 -0.1615373
C -2.0562774 2.9156464 0.3518779
N -2.4266339 4.1022093 0.8961313
C -4.2692801 1.8009267 0.5520003
C 0.2927145 3.5559464 -0.1486291
C -2.7443402 -0.4590740 -0.8829087
C 0.3240027 0.7195471 -1.3495743
H -2.0039318 -1.0799226 -1.3896376
H -3.5942748 -0.3324088 -1.5630027
H -3.0892596 -1.0067850 0.0015279
H 0.0836556 -0.2912483 -1.6826725
H 1.1647751 0.6496856 -0.6503167
H 0.6518719 1.2896594 -2.2263749
H -3.2952510 4.1390790 1.4132404
H -4.6528014 0.8081706 0.3251544
H -4.8494980 2.5439497 -0.0023131
H -4.3618587 1.9730242 1.6284325
H 0.6659819 3.6902983 0.8710782
H -0.0067374 4.5178282 -0.5735200
H 1.0859906 3.1330091 -0.7618799
H -1.7013581 4.7138731 1.2475474

4d-CO2_solv
E(TPSS-D3/def2-TZVP) = -627.8192230417 (conv)
Lowest Freq. = 66.55 cm^-1
26
4d-CO2_solv (021-CO2/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -0.4334863 -1.2406653 -0.4321720
C 0.8391637 -0.7915048 -0.6561187
N -1.0608343 -0.2862660 0.3753092
N 0.9764749 0.4087663 0.0475857
C -0.1870268 0.7063759 0.6627846
N -0.4210096 1.8002869 1.4407612
C -2.4461959 -0.3364614 0.8403576
C 2.1995047 1.2029434 0.1456430
C -1.1349489 -2.4680175 -0.8981224
C 1.9534182 -1.3717305 -1.4544143
H -0.4536677 -3.0761538 -1.4960539
H -2.0054236 -2.2226121 -1.5173064
H -1.4818272 -3.0728544 -0.0527498
H 1.6195728 -2.2914506 -1.9383629
H 2.8165560 -1.6125764 -0.8233153
H 2.2880747 -0.6763479 -2.2321941
H -1.0148710 1.6688270 2.2522737
H -3.0683375 -0.7503794 0.0466446
H -2.7735053 0.6796308 1.0626305
H -2.5259930 -0.9570275 1.7362150
H 2.1357898 1.8111222 1.0474331
H 2.2966374 1.8535821 -0.7245497
H 3.0496592 0.5228147 0.2132041
C -0.3959840 3.1764651 0.9037019
O 0.0483143 3.2890097 -0.2596148
O -0.8200547 4.0342234 1.7104304

4x_solv
E(TPSS-D3/def2-TZVP) = -478.4209274611 (conv)
Lowest Freq. = 16.89 cm^-1
26
4x_solv (002/c1/tpss-d3.def2-TZVP_COSMO_37.5)

C -2.0881918 0.8201623 -0.2789150
C -0.8113963 1.2493460 -0.4471073
N -2.8751293 1.9430477 0.0840722
N -0.8020697 2.6317558 -0.2086163
C -2.0775146 3.0908950 0.0853943
N -2.3053267 4.3557763 0.2970467
C -4.3330679 1.9284775 -0.0308211
H -4.6576948 2.2622842 -1.0235690
H -4.7865557 2.5604967 0.7295545
H -4.6765992 0.9055505 0.1254805
C 0.3381675 3.5256517 -0.2845091
H 0.3177639 4.1175757 -1.2075034
H 1.2555883 2.9367003 -0.2539371
H 0.3098579 4.2121494 0.5658432
C -3.5978517 4.8135138 0.7932087
H -3.5176995 5.8849853 1.0064005
H -3.8982876 4.3186456 1.7311805
H -4.4223132 4.6908403 0.0741158
C 0.4323597 0.4946207 -0.7681279
H 0.9080023 0.8692790 -1.6830228
H 0.1968679 -0.5614135 -0.9178350
H 1.1715760 0.5643647 0.0403368
C -2.6645865 -0.5507752 -0.3765735
H -3.4281683 -0.6263834 -1.1612187
H -3.1284173 -0.8663672 0.5670936
H -1.8711236 -1.2631790 -0.6143510

4x_vac
E(TPSS-D3/def2-TZVP) = -478.4099986798 (conv)
Lowest Freq. = 54.90 cm^-1
26
4x_vac (002/c1/tpss-d3.def2-TZVP)
C -2.0922131 0.8121329 -0.2840517
C -0.8209137 1.2497503 -0.4604537
N -2.8795025 1.9239378 0.1114801
N -0.8069842 2.6243524 -0.1995759
C -2.0854627 3.0853786 0.1145196
N -2.3115340 4.3348652 0.3398308
C -4.3270600 1.9258138 -0.0575647
H -4.6153436 2.1854712 -1.0856928
H -4.7890750 2.6317220 0.6289447
H -4.7052817 0.9272186 0.1701575
C 0.3259083 3.5208059 -0.3019987
H 0.5271167 3.8021591 -1.3439923
H 1.2177956 3.0511798 0.1222982
H 0.0674367 4.4215521 0.2582733
C -3.5767785 4.8168413 0.8557530
H -3.4566051 5.8740398 1.1136951
H -3.8985752 4.2946996 1.7733769
H -4.4042220 4.7582103 0.1297351
C 0.4256368 0.5069383 -0.7955792
H 0.9087141 0.9128804 -1.6933161
H 0.1981338 -0.5449243 -0.9826433
H 1.1597976 0.5523324 0.0198197
C -2.6606325 -0.5611394 -0.3783409
H -3.4459946 -0.6395366 -1.1418346
H -3.0949695 -0.8906485 0.5755349
H -1.8712016 -1.2680329 -0.6447551

4x-H_vac
E(TPSS-D3/def2-TZVP) = -478.8336503680 (conv)
Lowest Freq. = 73.28 cm^-1
27
4x-H_vac (002-H/c1/tpss-d3.def2-TZVP)
C -2.1210462 0.8088193 -0.3389075
C -0.8311143 1.2509583 -0.4154493
N -2.9356769 1.9449602 -0.2084808
N -0.8740268 2.6497030 -0.2907267

C -2.1609401 3.0522679 -0.1743928
N -2.6213693 4.3356728 -0.1056940
C -4.4001994 1.9525944 -0.2357323
H -4.7294583 2.9013025 -0.6623577
H -4.8094540 1.8279873 0.7703084
H -4.7400487 1.1330073 -0.8687337
C 0.2884452 3.5397425 -0.2900302
H 0.5494252 3.8370735 -1.3094072
H 1.1304997 3.0159899 0.1614310
H 0.0616755 4.4229426 0.3097757
C -3.3777361 4.8145940 1.0761085
H -3.8002646 5.7888008 0.8287179
H -2.7387039 4.9009888 1.9619896
H -4.1966628 4.1286993 1.2925276
C 0.4495742 0.5095154 -0.5807623
H 0.9932706 0.8416808 -1.4718914
H 0.2458377 -0.5565952 -0.6914577
H 1.1074324 0.6355091 0.2868194
C -2.6867544 -0.5678355 -0.3833208
H -3.3241548 -0.7172192 -1.2624607
H -3.2833403 -0.7836870 0.5097584
H -1.8774754 -1.2979224 -0.4314319
H -1.9684062 5.0203913 -0.4700093

4x-CO2_solv
E(TPSS-D3/def2-TZVP) = -667.1473493816 (conv)
Lowest Freq. = 36.79 cm^-1
29
4x-CO2_solv (002-CO2/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -2.0736369 0.8554382 -0.3962921
C -0.7592245 1.2337230 -0.3139722
N -2.8355307 2.0053333 -0.1833257
N -0.7491894 2.5963178 -0.0179960
C -2.0174810 3.0596495 0.0480465
N -2.4007795 4.3427857 0.3167748
C -4.2945752 2.0856509 -0.2396103
H -4.5711982 3.1237661 -0.4210643
H -4.7329305 1.7408909 0.6998166
H -4.6495039 1.4645151 -1.0624549
C 0.4415430 3.4203000 0.1710011
H 0.8449378 3.7188378 -0.7982763
H 1.1797186 2.8473269 0.7333714
H 0.1524795 4.3079198 0.7329394
C -3.2164440 4.6398987 1.5054673
H -2.7269648 5.4211721 2.0920928
H -3.2983756 3.7353504 2.1119941
H -4.2160520 4.9831491 1.2238108
C 0.4948020 0.4481205 -0.4760674
H 1.1151008 0.8543215 -1.2827430
H 0.2523360 -0.5878967 -0.7195298
H 1.0915876 0.4523655 0.4431619
C -2.6954048 -0.4710237 -0.6601964
H -3.3005925 -0.4554035 -1.5738792
H -3.3433951 -0.7777700 0.1684819
H -1.9161336 -1.2255488 -0.7820911
C -2.0622650 5.4049778 -0.6250844
O -2.4410872 6.5490937 -0.2810405
O -1.4434498 5.0297704 -1.6527389

4y_solv
E(TPSS-D3/def2-TZVP) = -714.4228698328 (conv)
Lowest Freq. = 30.09 cm^-1
44
4y_solv (027/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -0.3201750 -1.1604648 -0.6188271
C 0.9617237 -0.7260957 -0.5834860
N -1.1929158 -0.0820379 -0.2468623
N 0.9682867 0.6386638 -0.1746233

C -0.3622434 1.0803893 -0.2215573
N -0.6955003 2.3144061 -0.3809748
C -2.1128037 -0.3618582 0.9508739
C 2.1223674 1.5782421 -0.0272213
C -2.0498820 2.6631924 -0.7757898
H -1.9823460 3.3532398 -1.6278918
H -2.5815610 3.1983627 0.0206814
H -2.6573423 1.7952762 -1.0724784
C -0.8493083 -2.4747599 -1.0917313
C 2.1636593 -1.4964628 -1.0248843
C 3.4212639 0.8343668 0.3232508
H 3.8460814 0.2949858 -0.5235369
H 3.2686735 0.1401674 1.1554975
H 4.1534176 1.5846585 0.6370740
C 2.3161852 2.3745009 -1.3298629
H 3.1494718 3.0770233 -1.2173267
H 1.4059796 2.9310427 -1.5645947
H 2.5463702 1.6959939 -2.1586636
C -3.3789793 -1.0609502 0.4391503
H -3.8814650 -0.4282928 -0.2996025
H -4.0654362 -1.2304707 1.2762775
H -3.1608564 -2.0268639 -0.0200384
C -1.3621679 -1.2361142 1.9743285
H -0.4462858 -0.7321843 2.3009350
H -1.0928367 -2.2140551 1.5701053
H -2.0016898 -1.3939042 2.8490202
H -0.0487981 -3.0593405 -1.5519024
H -1.6370602 -2.3291256 -1.8408769
H -1.2747350 -3.0880733 -0.2870479
H 1.8309234 -2.4510638 -1.4378293
H 2.8515393 -1.7150158 -0.2026686
H 2.7270934 -0.9720292 -1.8044644
C 1.8340982 2.5193343 1.1591243
H 2.6750876 3.2117819 1.2689818
H 1.7421174 1.9361814 2.0821881
H 0.9168768 3.0851337 0.9987176
C -2.5320405 0.9234222 1.6759103
H -1.6717319 1.5418547 1.9450213
H -3.0437424 0.6269464 2.5968397
H -3.2292369 1.5175413 1.0860333

4y_vac
E(TPSS-D3/def2-TZVP) = -714.4164672347 (conv)
Lowest Freq. = 31.01 cm^-1
44
4y_vac (027/c1/tpss-d3.def2-TZVP)
C -0.3196029 -1.1628400 -0.6120784
C 0.9620913 -0.7288740 -0.5693885
N -1.1930515 -0.0892840 -0.2349240
N 0.9707591 0.6292489 -0.1449687
C -0.3623998 1.0753588 -0.2013226
N -0.6826496 2.3080651 -0.3523681
C -2.1164735 -0.3733823 0.9513369
C 2.1200825 1.5773243 -0.0278881
C -2.0227234 2.6886686 -0.7509977
H -1.9324245 3.3913414 -1.5896123
H -2.5461488 3.2235415 0.0513771
H -2.6445468 1.8380364 -1.0690570
C -0.8476640 -2.4701053 -1.1027998
C 2.1634973 -1.4976172 -1.0129609
C 3.4249321 0.8436558 0.3237598
H 3.8479454 0.2929711 -0.5169341
H 3.2811757 0.1611805 1.1674121
H 4.1579973 1.5990070 0.6225433
C 2.2950192 2.3532171 -1.3455144
H 3.1297364 3.0576617 -1.2571627
H 1.3818227 2.9065135 -1.5736203
H 2.5125331 1.6634445 -2.1685384

C -3.3777015 -1.0766485 0.4307910
H -3.8688581 -0.4509555 -0.3205782
H -4.0762948 -1.2399353 1.2592516
H -3.1557151 -2.0463147 -0.0183248
C -1.3725623 -1.2464344 1.9813365
H -0.4632925 -0.7387251 2.3190918
H -1.0896592 -2.2199192 1.5753645
H -2.0182526 -1.4147581 2.8497795
H -0.0492382 -3.0486310 -1.5742736
H -1.6360179 -2.3119075 -1.8483832
H -1.2714379 -3.0974001 -0.3071758
H 1.8327070 -2.4547051 -1.4214600
H 2.8561207 -1.7122053 -0.1933761
H 2.7232343 -0.9754571 -1.7972357
C 1.8406851 2.5411046 1.1427407
H 2.6865615 3.2299844 1.2382456
H 1.7488440 1.9762032 2.0772074
H 0.9281115 3.1108273 0.9728766
C -2.5471424 0.9114774 1.6705290
H -1.6926667 1.5348424 1.9453951
H -3.0687967 0.6180164 2.5870838
H -3.2384590 1.5019526 1.0700891

4y-H_vac
E(TPSS-D3/def2-TZVP) = -714.8428976070 (conv)
Lowest Freq. = 30.58 cm^-1
45
4y-H_vac (027-H/c1/tpss-d3.def2-TZVP)
C -0.1499672 -1.2605204 -0.2028309
C 1.1146964 -0.7666891 -0.3794438
N -0.9789590 -0.1930362 0.1943408
N 1.0545200 0.6272245 -0.1672010
C -0.2362421 0.9436667 0.1537180
N -0.7470970 2.1984812 0.3426879
C -2.3231133 -0.4104823 0.9130638
C 2.1619921 1.6802220 -0.2245080
C -1.6512882 2.7747301 -0.6781040
H -1.0891717 3.2757962 -1.4751459
H -2.3216961 3.4902437 -0.1983752
H -2.2421476 1.9742745 -1.1225242
C -0.6206794 -2.6406600 -0.5392806
C 2.3162193 -1.5785899 -0.7446711
C 3.4996625 1.0930650 -0.6908592
H 3.4488375 0.6992473 -1.7073000
H 3.8857540 0.3312465 -0.0145098
H 4.2153217 1.9190778 -0.6940298
C 1.7865629 2.7761271 -1.2417221
H 2.6693138 3.3973022 -1.4131067
H 0.9885552 3.4392016 -0.9089829
H 1.4967676 2.3288312 -2.1967096
C -3.3256773 -1.0142261 -0.0796338
H -3.4551169 -0.3546837 -0.9432973
H -4.2933594 -1.1090479 0.4207238
H -3.0378597 -2.0024276 -0.4359602
C -2.0360967 -1.3250396 2.1201797
H -1.3771628 -0.8124612 2.8272557
H -1.5799363 -2.2770879 1.8541506
H -2.9818839 -1.5358090 2.6262839
H 0.2401760 -3.2963172 -0.6701705
H -1.1772229 -2.6360827 -1.4831460
H -1.2573496 -3.0911454 0.2217867
H 2.0077095 -2.6188666 -0.8460299
H 3.0874581 -1.5456791 0.0282133
H 2.7637597 -1.2768150 -1.6936200
C 2.3731423 2.2305135 1.1969639
H 3.1592626 2.9899737 1.1713677
H 2.6898679 1.4293372 1.8706337
H 1.4838450 2.6968945 1.6315486

C -2.9352625 0.8727087 1.4926100
H -2.2619413 1.3887009 2.1763767
H -3.8132924 0.5486876 2.0590144
H -3.2838275 1.5669120 0.7291029
H -0.0687128 2.8635575 0.6898365

4y-CO2_solv
E(TPSS-D3/def2-TZVP) = -903.1535735229 (conv)
Lowest Freq. = 27.45 cm^-1
47
4y-CO2_solv (027-CO2/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -0.1206891 -1.2386399 0.0982914
C 1.1317872 -0.7766610 -0.2149647
N -0.9604563 -0.1272691 0.2196247
N 1.0601122 0.6179452 -0.2850863
C -0.2182234 0.9988938 0.0067037
N -0.6616945 2.2918498 0.1409823
C -2.4075673 -0.2062689 0.6983069
C 2.2765860 1.5206448 -0.4717140
C -1.2206470 3.0508814 -0.9804780
H -0.6289435 3.9523155 -1.1623408
H -2.2492560 3.3512012 -0.7624549
H -1.2084707 2.4230641 -1.8744227
C -0.5037430 -2.6752624 0.2542490
C 2.3366238 -1.6275392 -0.4583050
C 3.0767048 1.0388915 -1.6968269
H 2.4178548 0.9213840 -2.5627288
H 3.6141578 0.1086651 -1.5284752
H 3.8169430 1.8076656 -1.9336332
C 1.9112064 2.9844317 -0.7520399
H 2.8577477 3.4974224 -0.9460069
H 1.4281641 3.4796655 0.0884504
H 1.2924869 3.0825295 -1.6462616
C -3.1558769 -1.2641946 -0.1348154
H -3.0020083 -1.0892561 -1.2041430
H -4.2232339 -1.1601109 0.0773227
H -2.8738280 -2.2869322 0.1039139
C -2.3698149 -0.5465683 2.1959186
H -1.8417665 0.2439631 2.7362137
H -1.8743586 -1.4999961 2.3919210
H -3.3966762 -0.6119974 2.5682950
H 0.4038392 -3.2661892 0.3861096
H -1.0216098 -3.0582078 -0.6306004
H -1.1361861 -2.8498886 1.1256436
H 2.1494560 -2.6225944 -0.0518919
H 3.2318147 -1.2390846 0.0289841
H 2.5468193 -1.7413605 -1.5263473
C 3.0888433 1.4598755 0.8308943
H 3.9705266 2.0993778 0.7258865
H 3.4273987 0.4476396 1.0624586
H 2.4766654 1.8261827 1.6596453
C -3.1822211 1.1053139 0.5128959
H -2.8154277 1.9182640 1.1369827
H -4.2121354 0.8898130 0.8122296
H -3.2004674 1.4193548 -0.5326825
C -0.5595012 2.8947879 1.4494182
O -0.0635413 2.1551470 2.3411294
O -0.9779733 4.0761039 1.5270402

5a_solv
E(TPSS-D3/def2-TZVP) = -636.9672972462 (conv)
Lowest Freq. = 47.25 cm^-1
40
5a_solv (010/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -2.2643234 0.9990758 -1.2878080
C -0.9158404 1.1248753 -0.5577092
N -3.1285268 2.0669736 -0.7297528
N -0.9902319 2.4715154 0.0277475

C -2.1871823 3.0822997 -0.3283006
N -2.3573101 4.3565075 -0.3527280
C -4.0816851 1.5755934 0.3441573
C -5.1629541 0.7451632 -0.3608794
C -4.7552115 2.7615322 1.0422369
C -3.3698373 0.7225329 1.4143154
C 0.2578884 3.2072166 0.3670704
C 0.7744428 3.9711682 -0.8655236
C 1.3125651 2.1892580 0.8320505
C -0.0106039 4.1683780 1.5369264
C -3.5921174 4.9119970 -0.8854806
H -3.3311742 5.7305667 -1.5686267
H -4.2059644 5.3474184 -0.0862543
H -4.2008861 4.1742420 -1.4257757
H -2.1319711 1.1849640 -2.3583771
H -2.7191203 0.0164247 -1.1666209
H -0.7710030 0.3634066 0.2163006
H -0.0864554 1.0538753 -1.2695180
H -5.3552889 3.3449075 0.3408760
H -4.0197077 3.4198506 1.5143493
H -5.4187982 2.3742647 1.8219370
H -5.6736680 1.3551264 -1.1128044
H -5.8994957 0.3991063 0.3722482
H -4.7432176 -0.1372217 -0.8544674
H -2.9386051 -0.1881402 0.9872294
H -4.0927485 0.4194658 2.1792705
H -2.5732759 1.2962852 1.8982991
H -0.7559492 4.9143620 1.2599030
H 0.9243856 4.6688434 1.8115477
H -0.3732802 3.6078123 2.4056503
H 1.6165821 1.5111405 0.0295296
H 0.9371423 1.5959349 1.6725962
H 2.2007094 2.7346759 1.1659901
H 0.9818216 3.2752792 -1.6867995
H 1.7026605 4.5000218 -0.6219379
H 0.0253261 4.6962210 -1.1938168

5a_vac
E(TPSS-D3/def2-TZVP) = -636.9607048936 (conv)
Lowest Freq. = 50.97 cm^-1
40
5a_vac (010/c1/tpss-d3.def2-TZVP)
C -2.2691942 1.0025130 -1.2894543
C -0.9115219 1.1306657 -0.5698911
N -3.1317356 2.0599551 -0.7215894
N -0.9944489 2.4576140 0.0506519
C -2.1917901 3.0770668 -0.3173834
N -2.3482339 4.3465705 -0.3412696
C -4.0835169 1.5662948 0.3459205
C -5.1621070 0.7337211 -0.3612753
C -4.7594962 2.7551184 1.0368865
C -3.3740756 0.7165998 1.4210751
C 0.2525251 3.2048382 0.3712158
C 0.7573083 3.9577373 -0.8728697
C 1.3115216 2.1951235 0.8438781
C -0.0150482 4.1812835 1.5285906
C -3.5677753 4.9264611 -0.8735868
H -3.2860988 5.7467041 -1.5449587
H -4.1728841 5.3666138 -0.0705449
H -4.1858803 4.2048546 -1.4257207
H -2.1489860 1.1919336 -2.3612753
H -2.7177251 0.0160698 -1.1687554
H -0.7472058 0.3498009 0.1821555
H -0.0883765 1.0843012 -1.2934583
H -5.3494235 3.3388175 0.3274046
H -4.0259570 3.4125407 1.5123868
H -5.4326143 2.3746841 1.8119174
H -5.6574824 1.3366934 -1.1279413

H -5.9104642 0.3992625 0.3652603
H -4.7439292 -0.1578480 -0.8399425
H -2.9364621 -0.1928491 0.9964516
H -4.0961538 0.4073554 2.1844275
H -2.5814534 1.2932214 1.9070665
H -0.7554904 4.9274220 1.2407350
H 0.9216793 4.6805137 1.7999757
H -0.3812034 3.6334200 2.4038674
H 1.6141682 1.5053990 0.0502455
H 0.9419384 1.6126633 1.6946222
H 2.2018310 2.7435400 1.1664896
H 0.9627393 3.2568777 -1.6909337
H 1.6860925 4.4915045 -0.6428591
H 0.0040204 4.6778612 -1.2004648

5a-H_vac
E(TPSS-D3/def2-TZVP) = -637.3786304323 (conv)
Lowest Freq. = 32.06 cm^-1
41
5a-H_vac (010-H/c1/tpss-d3.def2-TZVP)
C -2.1390743 0.7260993 -0.8047165
C -0.8093815 0.9858832 -0.1039302
N -2.9795044 1.8953249 -0.4158640
N -0.8288955 2.4646009 0.0030234
C -2.1050608 2.8878925 -0.0828766
N -2.4663122 4.1713836 0.0981979
C -4.2848295 1.5704652 0.3157985
C -5.1175985 0.6920055 -0.6267059
C -5.1026155 2.8153214 0.6655753
C -3.9367017 0.8272417 1.6182558
C 0.4049866 3.3095672 0.2124165
C 0.4945705 4.4073233 -0.8640522
C 1.6405808 2.4079796 0.0701161
C 0.3957597 3.8906381 1.6387876
C -3.3977398 4.8942464 -0.7879274
H -2.8370317 5.6493524 -1.3471633
H -4.1839580 5.3792431 -0.2079234
H -3.8388257 4.1865412 -1.4880060
H -2.0259557 0.7184073 -1.8928767
H -2.6039752 -0.2053042 -0.4925169
H -0.7465729 0.5296871 0.8908641
H 0.0366491 0.6579622 -0.7033957
H -5.4537275 3.3355496 -0.2271477
H -4.5564450 3.5069006 1.3101434
H -5.9855585 2.4780868 1.2152839
H -5.3163253 1.2159975 -1.5659859
H -6.0743866 0.4664215 -0.1480213
H -4.6329242 -0.2614120 -0.8537287
H -3.3797027 -0.0959387 1.4340584
H -4.8591443 0.5531047 2.1379014
H -3.3501095 1.4680366 2.2850051
H -0.4369190 4.5770999 1.8273195
H 1.3185812 4.4525595 1.8062632
H 0.3414749 3.0887772 2.3806368
H 1.7353156 2.0047253 -0.9421459
H 1.6330049 1.5844579 0.7895929
H 2.5265721 3.0153758 0.2697711
H 0.4312374 3.9684959 -1.8636992
H 1.4622140 4.9075510 -0.7698448
H -0.2748328 5.1779020 -0.7768777
H -1.7475077 4.7482346 0.5145166

5a-CO2_solv
E(TPSS-D3/def2-TZVP) = -825.6822667967 (conv)
Lowest Freq. = 32.45 cm^-1
43
5a-CO2_solv (010-CO2/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -0.0755159 -2.1622614 -0.3909307

C 1.3796771 -1.6712812 -0.3601617
N -0.8655217 -0.9201033 -0.2610994
N 1.2499062 -0.2048513 -0.2303936
C -0.0447972 0.1329827 -0.1233719
N -0.4874948 1.4342949 0.0389675
C -2.3431174 -1.0331746 -0.0002406
C -2.8757126 -2.1766378 -0.8807731
C -3.1133763 0.2405095 -0.3658629
C -2.5393998 -1.3682645 1.4881146
C 2.4852600 0.6023939 0.0638506
C 2.3316516 2.0823967 -0.3042508
C 3.6253985 0.0191726 -0.7885062
C 2.8076689 0.4536187 1.5604820
C -0.7615596 2.2797866 -1.1258957
H -0.1211125 3.1660240 -1.1102277
H -1.8071397 2.5996122 -1.1240332
H -0.5616490 1.7074967 -2.0345305
H -0.3152784 -2.6586554 -1.3318428
H -0.3046294 -2.8380945 0.4364651
H 1.9371625 -2.0723735 0.4899307
H 1.9091787 -1.9184925 -1.2806637
H -2.9052157 0.5459937 -1.3947332
H -2.9020226 1.0701742 0.3087878
H -4.1796458 0.0063170 -0.2914608
H -2.6849941 -1.9778731 -1.9403393
H -3.9562896 -2.2477015 -0.7306733
H -2.4376908 -3.1420021 -0.6136291
H -2.0423486 -2.3085834 1.7488569
H -3.6086497 -1.4818855 1.6930142
H -2.1304973 -0.5664354 2.1082615
H 1.9804567 0.8402713 2.1611356
H 3.7202455 1.0134440 1.7886912
H 2.9787931 -0.5954892 1.8237417
H 3.3799181 0.0608038 -1.8546434
H 3.8584060 -1.0134103 -0.5153129
H 4.5220019 0.6203442 -0.6157532
H 2.0040378 2.1991464 -1.3407883
H 3.3187214 2.5444145 -0.2070368
H 1.6442290 2.6121435 0.3552821
C -0.6706431 1.9223194 1.3773457
O -0.3998928 1.0904042 2.2873315
O -1.0744983 3.1069291 1.4687011

5x_solv
E(TPSS-D3/def2-TZVP) = -400.9507362970 (conv)
Lowest Freq. = 61.77 cm^-1
22
5x_solv (004/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -2.1493947 0.6487487 -0.5827871
C -0.7113475 1.1330290 -0.7051828
N -2.8933063 1.9057499 -0.3734163
N -0.7310800 2.3010494 0.1780201
C -2.0110578 2.8641335 0.1534083
N -2.2065292 4.0823104 0.5287691
C -4.2316078 1.7011158 0.1906178
H -4.7517569 0.9736354 -0.4380557
H -4.8057919 2.6244264 0.1948931
H -4.1774747 1.3044072 1.2157001
C 0.4309648 3.1783552 0.1768681
H 0.5784782 3.6600003 -0.8027740
H 1.3172625 2.5859500 0.4194359
H 0.2907267 3.9534674 0.9309324
C -3.5197186 4.7041984 0.3981263
H -3.3878651 5.7902448 0.4486808
H -4.2086052 4.4257568 1.2093159
H -4.0104091 4.4715869 -0.5587766
H -2.5114267 0.1285813 -1.4730373
H -2.2680657 -0.0109545 0.2903250

H 0.0204203 0.3948815 -0.3684322
H -0.4734052 1.4257662 -1.7408008

5x_vac
E(TPSS-D3/def2-TZVP) = -400.9408616832 (conv)
Lowest Freq. = 68.58 cm^-1
22
5x_vac (004/c1/tpss-d3.def2-TZVP)
C -2.1488588 0.6428163 -0.5910636
C -0.7118497 1.1370565 -0.7161922
N -2.8988017 1.8888317 -0.3815826
N -0.7360104 2.2978864 0.1637895
C -2.0189427 2.8633870 0.1417072
N -2.2104224 4.0749175 0.5078498
C -4.2253748 1.6860203 0.1954729
H -4.7839522 1.0065645 -0.4557269
H -4.7703304 2.6247369 0.2606006
H -4.1665540 1.2364540 1.2003407
C 0.4172647 3.1812567 0.1858829
H 0.6329858 3.5988995 -0.8112195
H 1.2907078 2.6219164 0.5349422
H 0.2011572 4.0039028 0.8676680
C -3.5069723 4.7172019 0.4001916
H -3.3521536 5.8006098 0.4284043
H -4.1756492 4.4681639 1.2388651
H -4.0319593 4.4798201 -0.5385620
H -2.5059184 0.1162876 -1.4815757
H -2.2560796 -0.0229845 0.2813272
H 0.0237327 0.3988319 -0.3828401
H -0.4770086 1.4238628 -1.7564494

5x-H_vac
E(TPSS-D3/def2-TZVP) = -401.3531623325 (conv)
Lowest Freq. = 44.53 cm^-1
23
5x-H_vac (004-H/c1/tpss-d3.def2-TZVP)
C -2.1130910 0.5820250 -0.4710675
C -0.6740571 1.0677317 -0.6476068
N -2.8617396 1.8475344 -0.2785695
N -0.7133945 2.3660775 0.0514101
C -1.9924303 2.8039994 0.1138911
N -2.2767766 4.0489353 0.5095896
C -4.2846087 1.7384559 0.0698857
H -4.6943753 0.9145561 -0.5158774
H -4.8246886 2.6432258 -0.1982992
H -4.4181393 1.5198818 1.1356812
C 0.4531801 3.2458796 0.0766159
H 0.5057538 3.8823271 -0.8157089
H 1.3443477 2.6191960 0.1200068
H 0.4446154 3.8634484 0.9799342
C -3.5767357 4.7366830 0.5335825
H -3.3832802 5.7670562 0.8302947
H -4.2509029 4.2869440 1.2645899
H -4.0346425 4.7401748 -0.4584408
H -2.4984360 0.0503219 -1.3421771
H -2.2264562 -0.0482200 0.4198033
H 0.0606074 0.4069023 -0.1851314
H -0.4162490 1.2175115 -1.7036134
H -1.4700976 4.6247065 0.7097453

5x-CO2_solv
E(TPSS-D3/def2-TZVP) = -589.6640820685 (conv)
Lowest Freq. = 57.91 cm^-1
25
5x-CO2_solv (004-CO2/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -0.1952606 -2.1790311 -0.5628456
C 1.3002433 -1.8275527 -0.4678955
N -0.8309173 -0.9747626 0.0002777

N 1.2645446 -0.3608868 -0.3459339
C 0.0442887 0.0447653 0.0274347
N -0.2775593 1.3262032 0.3469507
C -2.1982801 -0.9589310 0.4941863
H -2.9190062 -0.8956168 -0.3284808
H -2.3272749 -0.1069150 1.1618714
H -2.3755454 -1.8803865 1.0547747
C 2.4386542 0.4732010 -0.5231229
H 2.9815711 0.1201257 -1.4040374
H 3.0842176 0.4291053 0.3590774
H 2.1190599 1.5040740 -0.6803421
C -1.4524335 1.9663327 -0.2674286
H -1.1388069 2.9224694 -0.6908551
H -2.2414338 2.1473216 0.4673639
H -1.8310025 1.3263913 -1.0663756
H -0.5249517 -2.3301021 -1.5968178
H -0.4621233 -3.0528713 0.0331133
H 1.7788433 -2.2660832 0.4154977
H 1.8586181 -2.1130718 -1.3603688
C 0.4686192 2.0564039 1.3926142
O 0.1274251 3.2532273 1.5163817
O 1.3085165 1.3765913 2.0249554

5y_solv
E(TPSS-D3/def2-TZVP) = -558.3065885361 (conv)
Lowest Freq. = 38.32 cm^-1
34
5y_solv (011/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -2.1316180 0.6488858 -0.6800579
C -0.6905016 1.1359119 -0.7509740
N -2.8854508 1.8974760 -0.4401064
N -0.7289062 2.2859035 0.1545316
C -2.0125263 2.8383432 0.1345805
N -2.2197895 4.0363620 0.5677045
C -4.2608347 1.7263278 0.1002905
C -5.0320042 0.7152298 -0.7499496
C -4.2494636 1.3415315 1.5856054
C 0.4355080 3.1828971 0.2556788
C 0.7068326 3.9331359 -1.0566459
C 1.6581900 2.3990507 0.7349208
C -3.5185871 4.6830852 0.4480803
H -3.3772714 5.7582024 0.6037000
H -4.2450563 4.3433901 1.2024290
H -3.9747436 4.5493066 -0.5445222
H -2.4563356 0.1649748 -1.6029773
H -2.2620867 -0.0531729 0.1551850
H 0.0218445 0.3811914 -0.4113678
H -0.4268784 1.4368035 -1.7760920
H -4.9990987 0.9917463 -1.8088253
H -6.0776788 0.6984012 -0.4278729
H -4.6305832 -0.2975994 -0.6391136
H -3.7743799 0.3667649 1.7418163
H -5.2754154 1.2830018 1.9641132
H -3.7066563 2.0901109 2.1725685
H 1.9847195 1.6691692 -0.0147660
H 1.4376209 1.8656714 1.6653701
H 2.4904428 3.0868553 0.9154163
H 1.0032463 3.2436023 -1.8551680
H 1.5192684 4.6542158 -0.9159869
H -0.1890549 4.4767058 -1.3722076
H -4.7621057 2.6879043 -0.0034259
H 0.1549940 3.9152037 1.0176086

5y_vac
E(TPSS-D3/def2-TZVP) = -558.2975621437 (conv)
Lowest Freq. = 39.31 cm^-1
34
5y_vac (011/c1/tpss-d3.def2-TZVP)

C -2.1346937 0.6419379 -0.6960742
C -0.6965762 1.1418790 -0.7850681
N -2.8935728 1.8818817 -0.4576947
N -0.7348083 2.2816322 0.1232268
C -2.0197549 2.8373158 0.1070527
N -2.2184840 4.0325432 0.5285417
C -4.2553743 1.7157239 0.1042507
C -5.0465431 0.7097713 -0.7339219
C -4.2250064 1.3342500 1.5910540
C 0.4206960 3.1822083 0.2523437
C 0.7218003 3.9344291 -1.0519265
C 1.6325122 2.4059048 0.7691382
C -3.5046452 4.6953675 0.4386563
H -3.3431492 5.7679256 0.5878116
H -4.2152930 4.3689837 1.2150082
H -3.9895694 4.5660324 -0.5418798
H -2.4646501 0.1478462 -1.6133309
H -2.2446885 -0.0603093 0.1440231
H 0.0270569 0.3903789 -0.4581621
H -0.4502298 1.4428937 -1.8164129
H -5.0291630 0.9878359 -1.7924500
H -6.0876638 0.6910126 -0.3971867
H -4.6470219 -0.3051380 -0.6324866
H -3.7615682 0.3531728 1.7434144
H -5.2436011 1.2897806 1.9914389
H -3.6586422 2.0757397 2.1633179
H 1.9881488 1.6756139 0.0323069
H 1.3857412 1.8735288 1.6930756
H 2.4578761 3.0952220 0.9739526
H 1.0377904 3.2490969 -1.8473125
H 1.5298952 4.6568142 -0.8939786
H -0.1671967 4.4791071 -1.3822880
H -4.7503040 2.6824265 0.0092986
H 0.1063228 3.9137810 1.0018018

5y-H_vac
E(TPSS-D3/def2-TZVP) = -558.7158555243 (conv)
Lowest Freq. = 42.99 cm^-1
35
5y-H_vac (011-H/c1/tpss-d3.def2-TZVP)
C -2.0954582 0.5867605 -0.5685485
C -0.6421307 1.0600790 -0.6207936
N -2.8495375 1.8368025 -0.3014873
N -0.6997635 2.3282939 0.1311902
C -1.9819264 2.7599133 0.1690963
N -2.2874632 3.9807443 0.6313637
C -4.2844870 1.7182473 0.1062367
C -5.0002068 0.7383552 -0.8230195
C -4.4044277 1.3272378 1.5826350
C 0.4806459 3.2275739 0.2052314
C 0.6722095 4.0124163 -1.0985655
C 1.7194050 2.4183624 0.5905121
C -3.5472138 4.7256724 0.5046463
H -3.3222984 5.7685824 0.7282523
H -4.2979895 4.3725736 1.2154946
H -3.9320855 4.6646053 -0.5158479
H -2.4245427 0.1352512 -1.5039485
H -2.2591265 -0.1219075 0.2511574
H 0.0453387 0.3585800 -0.1481448
H -0.3130969 1.2495187 -1.6494403
H -4.8659280 1.0156545 -1.8724958
H -6.0695605 0.7582938 -0.5983340
H -4.6523340 -0.2887136 -0.6767619
H -3.9788543 0.3358484 1.7673095
H -5.4594491 1.2947089 1.8689987
H -3.8961211 2.0483032 2.2310625
H 2.0134887 1.7355781 -0.2125842
H 1.5485872 1.8431691 1.5046434

H 2.5532797 3.1028596 0.7640836
H 0.9053462 3.3370690 -1.9274304
H 1.5068650 4.7106497 -0.9913174
H -0.2224876 4.5861747 -1.3603997
H -4.7303194 2.7002145 -0.0475468
H 0.2846679 3.9227956 1.0320507
H -1.4914967 4.5182942 0.9459790

5y-CO2_solv
E(TPSS-D3/def2-TZVP) = -747.0209142948 (conv)
Lowest Freq. = 24.05 cm^-1
37
5y-CO2_solv (011-CO2/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -0.2423763 -1.8013537 -0.8459114
C 1.2328014 -1.5005460 -0.5366785
N -0.9399212 -0.6763905 -0.1865963
N 1.1928674 -0.0661309 -0.1905305
C -0.0606901 0.3032169 0.0937142
N -0.4168035 1.5339314 0.5572959
C -2.3067780 -0.7876411 0.3579805
C -3.2930296 -1.1269678 -0.7612499
C -2.3501511 -1.8023732 1.5071337
C 2.3689770 0.8168842 -0.2729181
C 2.7900228 1.0049808 -1.7353373
C 3.4996488 0.2689381 0.5992962
C -1.5075388 2.2737599 -0.0973425
H -1.1440464 3.2713424 -0.3527777
H -2.3759223 2.3752143 0.5596358
H -1.7939400 1.7491358 -1.0108260
H -0.4531782 -1.7908819 -1.9197578
H -0.5682444 -2.7522976 -0.4255261
H 1.6099627 -2.0792764 0.3128281
H 1.8785780 -1.6663519 -1.3986900
H -3.2553595 -0.3770141 -1.5570247
H -4.3086896 -1.1580146 -0.3566708
H -3.0705712 -2.1082240 -1.1943235
H -2.1270623 -2.8147577 1.1548119
H -3.3536636 -1.8107244 1.9433822
H -1.6319454 -1.5327827 2.2871986
H 3.8513769 -0.6989927 0.2252371
H 3.1570404 0.1573851 1.6303770
H 4.3434104 0.9651130 0.5779944
H 3.1231906 0.0613789 -2.1803058
H 3.6236379 1.7124898 -1.7825692
H 1.9616845 1.4016546 -2.3303539
H -2.5430683 0.1976873 0.7624887
H 2.0404439 1.7754106 0.1299590
C 0.1779627 2.0905888 1.7890263
O 0.9544175 1.3282432 2.4069416
O -0.2075582 3.2515140 2.0538893

CO2_solv
E(TPSS-D3/def2-TZVP) = -188.6985839657 (conv)
Lowest Freq. = 641.60 cm^-1
3
CO2 (CO2/c1/tpss-d3.def2-TZVP_COSMO_37.5)
C -0.0000043 0.0000007 -0.0000010
O 0.0000021 -0.0000003 1.1684893
O 0.0000021 -0.0000003 -1.1684883

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