# Supporting Information

## Synergetic effects on the capture and release of $CO_2$ using guanidine and amidine superbases

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# Contents

# 1 General Information

$CO_2$ was sparged to improve $CO_2$ solubility for Table 1(MS), however greater amounts of SB were required for sparging and so the majority of data in supporting information was collected with $CO_2$ streamed at the surface of the solution.

## 2 Experiments

Solvents were purchased from Fisher Scientific and TCI Europe. Bases were obtained from Liuotin. CO2 was purchased from Woikoski, SFE grade (99.995%), and pumped directly into the reaction vessels.

Experiments were conducted under atmospheric conditions. All solutions were at a 30% wt concentration of superbase to solvent. Monoethanolamine (MEA) in industry is typically used around 30% due to constraints on machinery (corrosion issues). Our experiments modelled this value for comparison with industrial standards. Solvents were not dried deliberately to test the hardiness of the systems. The carbon dioxide stream used was also not dried beforehand for the same reason. To establish the $CO_2$ release temperature for every superbase solvent combination, an initial experiment was carried out. Table S1 presents the solvents originally chosen for this study that were mixed with the 8 different superbases used.

Experimental method for establishing $CO_2$ release temperature: 10g of superbase-solvent solution was stirred in a flask with a stream of carbon dioxide directed at the surface for 5 minutes. The $CO_2$ exposed solution was then placed in a preheated oil bath at 60°C. Whilst stirring the temperature was incrementally increased until bubbles started to form, observing the carbon dioxide being released. The time the solution produced bubbles for was also noted. The temperature was increased up until the boiling point of the solvent.

Experimental method for quantifying the amount of $CO_2$ released: 10g of superbase-solvent solution was stirred in a flask with a stream of carbon dioxide directed at the surface for 15 minutes. The $CO_2$ exposed solution was then placed in a preheated oil bath at the SB-solvent $CO_2$ release temperature, established in table S2. However, when the flask was placed in the oil bath for reversal, a tube was fitted to the flask to redirect the released gas into a manual burette system to capture and measure the gas produced.

$CO_2$ capture capacity from repeated capture/release cycles: The superbase-solvent solution was exposed to five capture and release cycles of $CO_2$ using a manual burette system to verify the reproducibility and hardiness of the system. 10g of superbase-solvent solution was stirred in a flask with a stream of carbon dioxide directed at the surface for 15 minutes. The $CO_2$ exposed solution was then placed in a preheated oil bath at the SB-solvent CO2 release temperature, established in table S2. However, when the flask was placed in the oil bath for reversal, a tube was fitted to the flask to redirect the released gas into a manual burette system to capture and measure the gas produced. After reversal the flask was disconnected from the burette and then this process was performed again, for a total of 5 times.

Experimental method for results in MS Table 1: 30g of superbase-solvent solution was stirred in a flask and carbon dioxide was sparged through the solution for 30 minutes. The $CO_2$ exposed solution was then placed in a preheated oil bath at the established SB-solvent $CO_2$ release temperature and a tube was fitted to the flask to redirect the released gas into a manual burette system to capture and measure the gas produced. Results are presented in Table 1 in the manuscript.

**Table S1**. Solvents used in study and comparative rating on how green they are. R=recommended, P= problematic and H=hazardous.

| Solvent | classification | Green | BP (°C) | Polarity Index (P′) | dielectric constant |
|---|---|---|---|---|---|
| Ethanol | alcohol | R | 78 | 4.3 | 24.55 |
| Ethyl acetate | ester | R | 77 | 4.4 | 6.02 |
| n-Butyl acetate | ester | R | 126 | 4 | 5.01 |
| THF | ether | P | 66 | 4 | 7.58 |
| 1,4-dioxane | ether | H | 101 | 4.8 | 2.21 |
| Toluene | hydrocarbon | P | 111 | 2.4 | 2.38 |
| Cyclohexane | hydrocarbon | P | 81 | 0.2 | 2.02 |
| Acetonitrile | polar aprotic | P | 82 | 5.8 | 35.94 |
| Propylene carbonate | polar aprotic | P | 242 | 6.1 | 64.92 |
| water | water | R | 100 | 10.2 | 78.36 |

Table S2 presents the data on which temperature the superbase-solvent mixtures released carbon dioxide at, and how long it took for no more carbon dioxide to be released. It also includes reversibility, and miscibility information. 30% wt concentration solutions were used, where the superbase was 3g in weight. 10g of superbase-solvent solution was stirred in a flask with a stream of carbon dioxide directed at the surface for 5 minutes. The $CO_2$ exposed solution was then placed in a preheated oil bath at 60°C. While stirred the temperature was incrementally increased until bubbles started to form, observing the carbon dioxide being released. The time the solution produced bubbles for was also noted. The temperature was increased up until the boiling point of the solvent, observing an increase in gas release.

All solutions formed a white-ish precipitate apart from water and ethanol. Upon release of $CO_2$ the precipitate disappears.

**Table S2** Superbases in different solvents and the temperature at which $CO_2$ is released. [a] mixture is irreversible or only partially reversible,

| | DBU | | DBN | | TMG | | TBN | | TBU | | TBD | | mTBD | | mTBN | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Solvent | Reversibility temperature (°C) | Time CO2 release (min) | Reversibility temperature (°C) | Time CO2 release (min) | Reversibility temperature (°C) | Time CO2 release (min) | Reversibility temperature (°C) | Time CO2 release (min) | Reversibility temperature (°C) | Time CO2 release (min) | Reversibility temperature (°C) | Time CO2 release (min) | Reversibility temperature (°C) | Time CO2 release (min) | Reversibility temperature (°C) | Time CO2 release (min) |
| Ethanol | 60 | 11 | 65 | 14 | 75 | 20 | 76 | 45 | 60 | 10 | 63 | 13.5 | 64 | 11 | 67 | 20 |
| Ethyl acetate | 68 | 4 | 60 | 4.5 | 70 | 2 | 77[a] | 4[b] | 60[a] | 16[a,c] | 61 | 11 | 72 | 18 | 60 | 3 |
| n-Butyl acetate | 80 | 2 | 60 | 8 | 65 | 4 | 90[a] | 12[a,c] | 62[a] | 15[a,c] | 83 | 11.5 | 65 | 13 | 60 | 6.5 |
| THF | 60 | 20 | 60 | 11 | 75 | 2 | 70 | 9[b] | 60 | 9 | 61 | 3.5[b] | 60[a] | [a,c] | 60 | 8 |
| 1,4-dioxane | 75 | 5 | 60 | 12 | 65 | 7 | [a] | [a] | 88[a] | 9[a,c] | 90[a] | 15.5[a,c] | 60 | 11.5 | 62 | 8.5 |
| Cyclohexane | 70 | 5 | 60 | 14 | 66 | 8 | 70[a] | 15[a,c] | 80[a] | [a,c] | 73[a] | 5.5[a,c] | 65 | 15 | 60 | 10 |
| Toluene | 70 | 7 | 60 | 10 | 65 | 7 | [a] | [a,b] | 109[a] | [a,c] | 91 | 4.5[b] | 60 | 9 | 60 | 10 |
| Acetonitrile | 60 | 4 | 60 | 10.5 | 62 | 6 | 68[a] | [a] | 60 | 12[b] | 60 | 13.5[b] | 60 | 7 | 60 | 10 |
| Propylene carbonate | 65 | 2 | 60 | 12 | 60 | 7 | 106[a] | 2[a,c] | 85[a] | 48[a,c] | 114 | 48[b] | 68 | 7 | 75 | 12.5 |

[b] superbase is miscible in solvent at 30°C, [c] superbase is miscible at 50°C

Table S3 presents data for the molar ratio of superbase to $CO_2$ for the best five solvents. 10 g of 30% wt superbase-solvent solution was stirred with a direct stream of $CO_2$ at the surface for 15 minutes. After which the flask had a tube was fitted that was connected to a manual burette system to collect the $CO_2$ gas that was evolved for quantification. The flask was the submerged in an oil bath at the, now established, $CO_2$ release temperature. TMG and TBU were not included; TMG has longer-term stability issues and TBU had solubility issues after the $CO_2$ release process.

**Table S3.** SB-solvent combinations and the molar ration of SB-$CO_2$ captured. [a] an irreversible reaction meaning severely diminished or no $CO_2$ generated [b] A side reaction deactivates the guanidine from capturing $CO_2$ after 1 regeneration cycle.

| Solvent | DBU $CO_2$/SB mol/mol | DBN $CO_2$/SB mol/mol | TBN $CO_2$/SB mol/mol | TBD $CO_2$/SB mol/mol | mTBN $CO_2$/SB mol/mol | mTBD $CO_2$/SB mol/mol |
|---|---|---|---|---|---|---|
| ethanol | 0.123 | 0.185 | 0.048 | 0.035 | 0.154 | 0.044 |
| ethyl acetate | 0.084 | 0.156 | [a] | 0.018 | 0.101 | 0.042 |
| butyl acetate | 0.094 | 0.072 | 0.312 | 0.015 | 0.094 | 0.091 |
| acetonitrile | 0.064 | 0.307 | [a] | 0.211 | 0.161 | 0.050 |
| propylene carbonate | 0.139 | 0.103 | 0.236 | [b] | 0.130 | 0.071 |

[a] An irreversible reaction meaning severely diminished or no $CO_2$ generated

[b] A side reaction deactivates the guanidine from capturing $CO_2$ after 1 regeneration cycle.

Table S4 compared the data for the molar ratio of superbase to $CO_2$ in absence of water for the release of $CO_2$ with the presence of water for two best candidates in their respective solvent. In this procedure 1 mL of water was added forcing the formation of the bicarbonate specie.

**Table S4** Comparison of adding 1ml water on the release volume of $CO_2$

| DBN | | TBN | |
|---|---|---|---|
| No water $CO_2$/SB mol/mol | 1ml water $CO_2$/SB mol/mol | No water $CO_2$/SB mol/mol | 1ml water $CO_2$/SB mol/mol |
| 0.306 | 0.305 | 0.312 | 0.311 |

## 2.1 Experimental work schematic

## 2.2 Design of Experiment

Design of Experiment surface plot using a quadratic, full factorial model. 3 centre points, and 30 total runs, reproducibility of 0.99 and R2 of 0.823. The software used was MODDE Pro, made by Sartorius.

# 3 Computational Details

## 3.1 Methodology

All DFT calculation were carried out using Gaussian 16 [1]. We applied the default ultrafine grid and the default optimization algorithms. All geometries were fully optimized in acetonitrile (MeCN) or in butyl acetate (BuOAc), using the ωB97X-D functional [2], and the 6-311G(d,p) basis set [3]. The solvent effects were taken into account implicitly via the SMD solvation model [4]. The located structures were characterized as energy minima or transition states (TSs) based on the number of imaginary vibrational frequency (zero or one). From the TSs, we followed the intrinsic reaction coordinate (IRC) pathways in both forward and reverse directions, using a Hessian-based predictor-corrector algorithm [5] and we identified the related intermediates accordingly.

The thermal and entropic corrections were also estimated at this level of theory (i. e., in the solution-phase, ωB97X-D/6-311G(d,p)) and within Grimme's quasi rigid rotor harmonic oscillator approximation (q-RRHO) [6]. The Gibbs free energies were calculated at room temperature (298.15 K) and were corrected to the standard 1 mol/dm$^3$ concentration.

In order to estimate the electronic energy more accurately, we calculated the gas-phase electronic energy with the LNO-CCSD(T) method [7] and added the solvation free energy and the thermal and entropic corrections to this electronic energy. The sum of these corrections was estimated by subtracting the gas phase electronic energy calculated at the level of optimization (ωB97X-D/6-311G(d,p)) from the sum of solution-phase electronic energy and thermal and entropic corrections. The total Gibbs free energy of a structure was calculated according to equation 1, where $E^{'}_{\circ}$ is the the LNO-CCSD(T)/CBS electronic energy, $\Delta G^{solv}_{\circ}$ is the entropic and solvation correction, and $\Delta G_{conc}$ is the concentration correction.

$$G = E^{'}_{\circ} + \Delta G^{solv}_{\circ} + \Delta G_{conc} \quad (1)$$

The LNO-CCSD(T) calculations were carried out with the MRCC program [8]. The CCSD(T) correlation energy was extrapolated as

$$E_{\mathrm{N-T}} = E_{\mathrm{T}} + \frac{E_{\mathrm{T}} - E_{\mathrm{N}}}{2} \quad (2)$$

where N and T refer to "normal" and "tight" composite cutoff thresholds offered by the MRCC program. The LNO-CCSD(T) calculations were carried out using the correlation consistent

basis set developed by Dunning [9]. The complete basis set limit of the LNO-CCSD(T) energies were estimated relying on extrapolation techniques employing the aug-cc-pVTZ and aug-cc-pVQZ basis sets. From the results with the aug-cc-pVTZ (TZ) and the aug-cc-pVQZ (QZ) basis sets, we extrapolated towards the complete basis set (CBS) limit of the Hartree-Fock and the correlation energy according to [10]:

$$E_{\mathrm{CBS}}^{\mathrm{HF}} = E_{\mathrm{QZ}}^{\mathrm{HF}} + \frac{5\left(E_{\mathrm{QZ}}^{\mathrm{HF}} - E_{\mathrm{TZ}}^{\mathrm{HF}}\right)}{4\exp\left[6.57(\sqrt{4}-\sqrt{3})\right]} \tag{3}$$

$$E_{\mathrm{CBS}}^{\mathrm{C}} = \frac{3^3 E_{\mathrm{TZ}}^{\mathrm{C}} - 4^3 E_{\mathrm{QZ}}^{\mathrm{C}}}{3^3 - 4^3} \tag{4}$$

We estimated the CCSD(T)/CBS limit by extrapolating towards the CCSD(T) limit on the TZ basis and extrapolating towards the CBS limit with the normal threshold. The final LNO-CCSD(T)/CBS energies were calculated according to the following formula:

$$E_{\mathrm{CCSD(T)}}^{\mathrm{CBS}} = E_{\mathrm{N}}^{\mathrm{CBS}} + E_{\mathrm{N-T}}^{\mathrm{TZ}} - E_{\mathrm{N}}^{\mathrm{TZ}} \tag{5}$$

where $E_{\mathrm{N}}^{\mathrm{CBS}}$ is the sum of $E_{\mathrm{CBS}}^{\mathrm{HF}}$ and $E_{\mathrm{CBS}}^{\mathrm{C}}$, whereas $E_{\mathrm{N-T}}^{\mathrm{TZ}}$ and $E_{\mathrm{N}}^{\mathrm{TZ}}$ refer to CCSD(T) correlation energies. The correlation of the core electrons was neglected.

Conformational search was carried out for all bases, complexes and transition states with the Macromodel utility of the Schrödinger program [11] and the OPLS_2005 force field [12]. The promising structures were optimized with DFT and the most stable ones are presented.

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## 3.2 $CO_2$ capture in acetonitrile

### 3.2.1 $CO_2$ capture with **DBN**

The $CO_2$ capture was first studied with the superbase 1,5-Diazabicyclo[4.3.0]non-5-ene (**DBN**). It was found that $CO_2$ may form a weakly bounded precomplex with **DBN**, from which the zwitterionic adduct is formed through a relatively low barrier (Figure S1). The formation of the adduct from the precomplex is not favoured in terms of gas phase electronic energies (LNO-CCSD(T), green numbers in Figure S1) but is favoured in terms of Gibbs free energy as the polar solvent stabilizes the zwitterionic structure. The overall process is predicted to be slightly endergonic (1.1 kcal/mol).

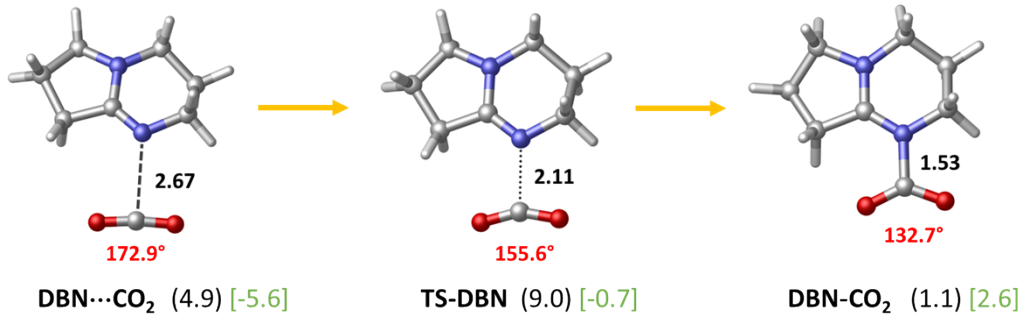



**Figure S1.** Structures for the $CO_2$ capture with **DBN** in acetonitrile. N-C distances are given in Å and C-O-C bond angles are given in degrees. Gibbs free energies (black) and gas phase electronic energies (green) with respect to separated reactants are presented in kcal/mol.

### 3.2.2 $CO_2$ capture with **TBN**

Next, we studied the $CO_2$ capture with 1,5,7-triazabicyclo(4.4.0)dec-5-ene (**TBN**). The reaction proceeds analogously to DBN, but the formation of the adduct is exergonic in this case

(-4.5 kcal/mol). This difference originates from the N-H···O hydrogen bond in **TBN-$CO_2$** (Figure S2). This interaction is negligible in the precomplex and the transition state.

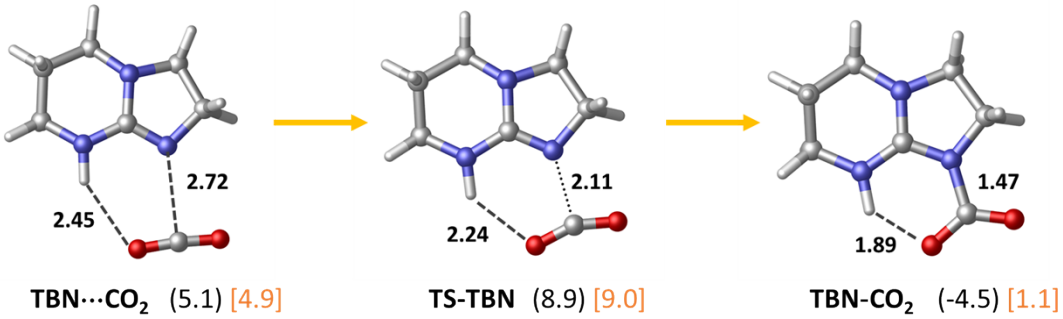
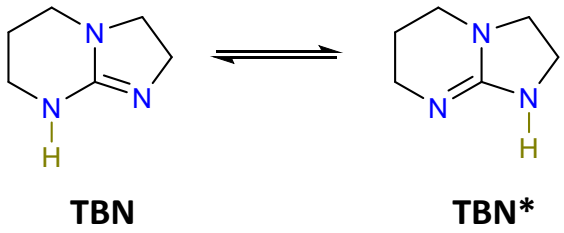



**Figure S2.** Structures for the $CO_2$ capture with **TBN** in acetonitrile. Selected bond distances are given in Å. Gibbs free energies (black) are given in parenthesis in kcal/mol with respect to separated reactants. The analogous stabilites with **DBN** are written in squared brackets (orange).

It is possible that the envisioned structure of **TBN** tautomerizes and the tautomer may also act as a superbase (Scheme S1). For this reason, we also studied the $CO_2$ capture with the **TBN** tautomer (denoted as **TBN***). The stability of TBN* with respect to TBN is 0.8 kcal/mol. This difference is reflected in the stability of the precomplex (5.7 kcal/mol instead of 5.1 kcal/mol) but not in the transition state (9.0 kcal/mol instead of 8.9 kcal/mol). The stability of the adduct is lower (-2.4 kcal/mol instead of -4.5 kcal/mol), which is evidenced by the elongated C-N bond in **TBN*-$CO_2$** (Figure S1).




**Scheme S1**. The tautomerization of **TBN**.

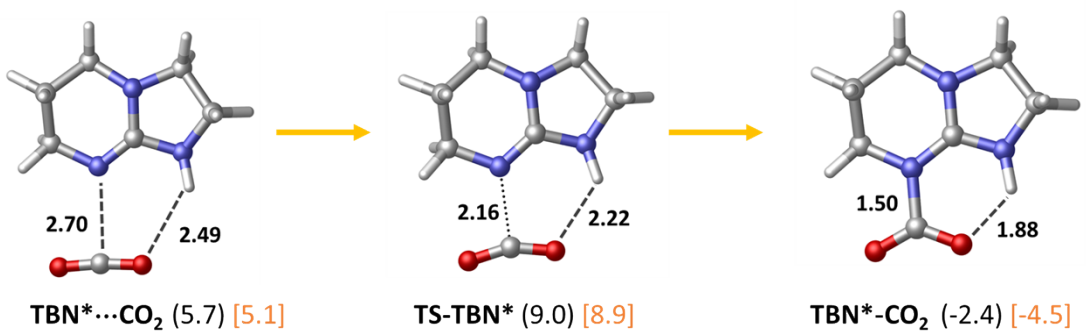



**Figure S3.** Structures for the $CO_2$ capture with **TBN*** in acetonitrile. Selected bond distances are given in Å. Gibbs free energies (black) are given in parenthesis in kcal/mol with respect to separated reactants. The analogous stabilites with **TBN** are written in squared brackets (orange).

### 3.2.3 $CO_2$ capture with **MTBN**

The capture of $CO_2$ was also investigated with the methylated **TBN** (7-Methyl-1,5,7-triazabicyclo(4.4.0)dec-5-ene, **MTBN**). The adduct formation again proceeds in a similar manner to **DBN**, but in this case, the barrier is notably higher (13.5 kcal/mol) and the adduct is unstable (lies 6.2 kcal/mol higher than separated reactants). The structures are depicted in Figure S4. It is clear that the adduct formation becomes unfavoured due to the repulsion between the $CO_2$ and the methyl group of **MTBN**. In order to avoid the steric hindrance, the orientation of the $CO_2$ group differs from the ideal arrangement. This strain also increases the barrier.

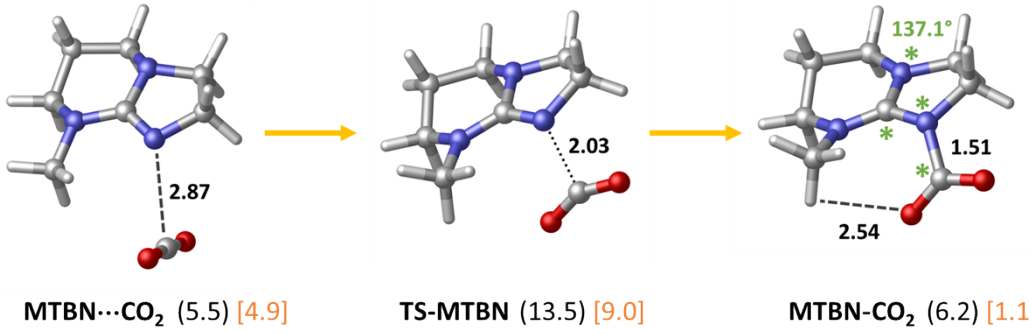



**Figure S4.** Structures for the $CO_2$ capture with **MTBN** in acetonitrile. Selected bond distances are given in Å. The dihedral angle corresponding to the atoms marked with * is presented with green. Gibbs free energies (black) are given in parenthesis in kcal/mol with respect to separated reactants. The analogous stabilites with **DBN** are written in squared brackets (orange).

## 3.3 $CO_2$ capture in butyl acetate

All structures were reoptimized in butyl acetate, but the geometries only show marginal differences if we compare them in the two solvents. A few structures are compared in Figure S5. The energetics, however, changes significantly if we move to another solvent (Table S5).

This is due to the different polarity of the two solvents as the less polar butyl acetate stabilizes the adducts and the transition states to a lower extent.

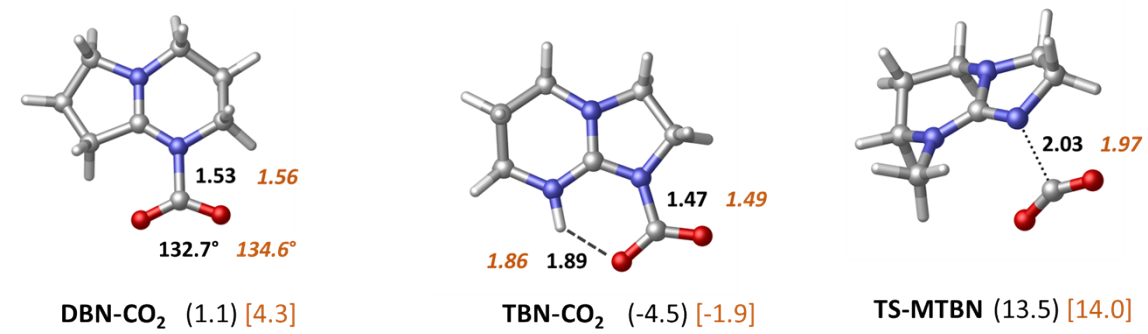



**Figure S5.** Structures for the $CO_2$ capture with various bases in acetonitrile. Selected bond distances are given in Å for the structures in acetonitrile and the analogous values in the butyl acetate structures are written in orange (with italics). Gibbs free energies are given in parenthesis in kcal/mol with respect to separated reactants (black for acetonitrile and orange for butyl acetate).

**Table S5.** Gibbs free energies of base-$CO_2$ weakly bounded complexes (B···$CO_2$) transition states (TS) and zwitterionic adducts (B-$CO_2$) with respect to separated reactants (B + $CO_2$) in different solvents [kcal/mol].

| | DBN | | TBN | | TBN* | | mTBN | |
|---|---|---|---|---|---|---|---|---|
| | MeCN | BuOAC | MeCN | BuOAC | MeCN | BuOAC | MeCN | BuOAC |
| B + $CO_2$ | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| B···$CO_2$ | 4.9 | 4.3 | 5.1 | 3.9 | 4.8 | 4.3 | 5.5 | 4.9 |
| TS | 9.0 | 8.7 | 8.9 | 8.2 | 8.2 | 7.7 | 13.5 | 14.0 |
| B-$CO_2$ | 1.1 | 4.3 | -4.5 | -1.9 | -3.2 | -0.7 | 6.2 | 9.9 |

### 3.4 Carbonate formation

In case water is added to the solutions, it is possible that it assists the capture of carbon-dioxide. In this case, hydrogen-carbonate could be formed. This hypothesis was investigated with the base **TBN**.

Initially, $H_2O$ forms a hydrogen bond with the base and $CO_2$ may coordinate to this complex (Figure S6). $CO_2$ is weakly bonded in this precomplex, no significant interaction is observed either with water or **TBN**. In **TS-TBN-$H_2O$**, a bond is being formed between the oxygen of the water molecule and the carbon of $CO_2$, and $H_2O$ is being deprotonated. The barrier is notably larger than it was without water (19.2 kcal/mol instead of 8.9 kcal/mol in acetonitrile), but the reaction remains feasible at room temperature. Once the product is formed, it spontaneously rearranges so that the formation of stronger hydrogen bonds is possible. This rearrangement makes the otherwise slightly endergonic process (1.9 kcal/mol in MeCN and 3.8 kcal/mol in BuOAc) slightly exergonic (-1.5 kcal/mol and -1.0 kcal/mol respectively).

However, the formation of the adduct is still less favoured than the formation of **TBN-$CO_2$** (-4.5 kcal/mol and -1.9 kcal/mol, see table S5).

These results imply that the formation a $HCO_3^-$-base-$H^+$ adduct is feasible in case water is added, but it is unfavoured both kinetically and thermodynamically as compared to the formation of the base-$CO_2$ adduct. This conclusion is in agreement with the experimental observation that the addition of water does not change the results significantly.

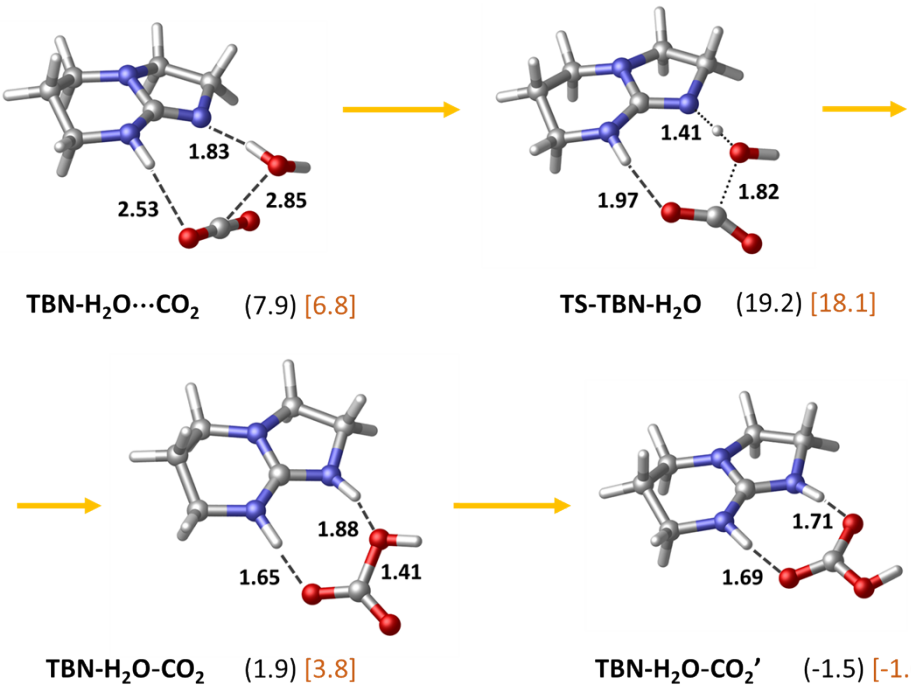



**Figure S6.** Structures for the $CO_2$ capture with **TBN-$H_2O$**. Selected bond distances are given in Å for the structures in acetonitrile. Gibbs free energies are given in parenthesis in kcal/mol with respect to separated reactants (black for acetonitrile and orange for butyl acetate).

### 3.5 Proton affinities

We calculated the proton affinity of each base discussed so far to demonstrate that the different feasibility of the $CO_2$ capture originates from specific interactions with the carbon-dioxide and not from the different intrinsic basicity of the various bases. The proton affinity was calculated as the Gibbs free energy of the following reaction:

$$\text{base} + H^+ \longrightarrow \text{base-}H^+$$

The proton affinities in both solvents are collected into Table S6. The values differ no more than 1.3 kcal/mol in MeCN and no more than 1.0 kcal/mol in BuOAc. In contrast, the stability

of the CO2-base adducts vary from -4.5 kcal/mol to 6.2 kcal/mol in MeCN and from -1.9 kcal/mol to 9.9 kcal/mol in BuOAc (see Table S5). This implies that their different stability originates from secondary interactions between $CO_2$ and the bases. In case of TBN and TBN*, a strong hydrogen bond can be observed (Figures S2 and S3), whereas with MTBN, a steric repulsion between the $CO_2$ and the methyl group decreases the stability (Figure S4).

**Table S6.** Proton affinities for the bases of interest in acetonitrile (MeCN) and butyl acetate (BuOAc) [kcal/mol].

| base | MeCN | BuOAc |
|---|---|---|
| DBN | -293.6 | -286.0 |
| TBN | -292.6 | -285.3 |
| TBN* | -293.4 | -286.0 |
| MTBN | -292.3 | -285.0 |

### 3.6 Total energy data

We present the calculated energies of the introduced structures in **Table S7**. For each structure, the first number is the Gibbs free energy calculated at the level of optimization (ωB97X-D/6-311G(d,p), solution-phase, quasi-RRHO approximation). Then gas-phase electronic energy is included first calculated at the same level of theory, and then with the LNO-CCSD(T) method. The final data is the calculated total Gibbs-free energy of the structure, which includes the concentration correction to the free energy when switching from $p$ = 1 atm (ideal gas standard state) to $c$ = 1 mol/dm$^3$. For computational details, see earlier.

**Table S7.** Total energy data.

| | $G_0$ | $E_0^{DFT}$ | $E_0^{CC}$ | $G$ |
|---|---|---|---|---|
| | | **MeCN** | | |
| **$CO_2$** | -188.5859 | -188.5767 | -188.4206 | -188.4267 |
| **$H_2O$** | -76.4273 | -76.4233 | -76.3773 | -76.3783 |
| **DBN** | -383.3067 | -383.4461 | -382.9775 | -382.8350 |
| **DBN-H** | -383.7837 | -383.8640 | -383.3863 | -383.3030 |
| **DBN---$CO_2$** | -571.8838 | -572.0337 | -571.4070 | -571.2540 |
| **DBN-TS** | -571.8787 | -572.0274 | -571.3992 | -571.2475 |
| **DBN-$CO_2$** | -571.8885 | -572.0193 | -571.3938 | -571.2599 |
| **TBN** | -399.3623 | -399.4860 | -399.0189 | -398.8923 |

| | | | | |
|---|---|---|---|---|
| **TBN-H** | -399.8394 | -399.9039 | -399.4260 | -399.3585 |
| **TBN---$CO_2$** | -587.9389 | -588.0747 | -587.4496 | -587.3108 |
| **TS-TBN** | -587.9348 | -588.0692 | -587.4421 | -587.3048 |
| **TBN-$CO_2$** | -587.9540 | -588.0697 | -587.4449 | -587.3262 |
| | | | | |
| **TBN-$H_2O$---$CO_2$** | -664.3644 | -664.5172 | -663.8405 | -663.6847 |
| **TS-TBN-$H_2O$** | -664.3513 | -664.5012 | -663.8196 | -663.6667 |
| **TBN-$H_2O$-$CO_2$** | -664.3769 | -664.5116 | -663.8320 | -663.6943 |
| **TBN-$H_2O$-$CO_2$'** | -664.3828 | -664.5268 | -663.8466 | -663.6996 |
| | | | | |
| **TBN*** | -399.3616 | -399.4853 | -399.0177 | -398.8909 |
| **TBN*---$CO_2$** | -587.9389 | -588.0743 | -587.4484 | -587.3100 |
| **TS-TBN*** | -587.9349 | -588.0702 | -587.4430 | -587.3047 |
| **TBN*-$CO_2$** | -587.9506 | -588.0687 | -587.4440 | -587.3228 |
| | | | | |
| **MTBN** | -438.6412 | -438.7925 | -438.2716 | -438.1173 |
| **MTBN-H** | -439.1173 | -439.2120 | -438.6808 | -438.5830 |
| **MTBN---$CO_2$** | -627.2171 | -627.3778 | -626.6990 | -626.5352 |
| **TS-MTBN** | -627.2063 | -627.3658 | -626.6849 | -626.5224 |
| **MTBN-$CO_2$** | -627.2152 | -627.3555 | -626.6774 | -626.5341 |
| | | | | |
| | | **BuOAc** | | |
| **$CO_2$** | -188.5868 | -188.5767 | -188.4206 | -188.4277 |
| **$H_2O$** | -76.4255 | -76.4233 | -76.3774 | -76.3765 |
| | | | | |
| **DBN** | -383.3041 | -383.4463 | -382.9776 | -382.8324 |
| **DBN-H** | -383.7689 | -383.8640 | -383.3863 | -383.2881 |
| **DBN---$CO_2$** | -571.8830 | -572.0338 | -571.4069 | -571.2531 |
| **DBN-TS** | -571.8775 | -572.0266 | -571.3983 | -571.2462 |
| **DBN-$CO_2$** | -571.8822 | -572.0211 | -571.3951 | -571.2532 |
| | | | | |
| **TBN** | -399.3588 | -399.4861 | -399.0190 | -398.8886 |
| **TBN-H** | -399.8242 | -399.9040 | -399.4261 | -399.3433 |
| **TBN---$CO_2$** | -587.9384 | -588.0749 | -587.4497 | -587.3101 |
| **TS-TBN** | -587.9336 | -588.0688 | -587.4414 | -587.3032 |
| **TBN-$CO_2$** | -587.9474 | -588.0711 | -587.4460 | -587.3193 |
| | | | | |
| **TBN-$H_2O$---$CO_2$** | -664.3624 | -664.5185 | -663.8411 | -663.6819 |
| **TS-TBN-$H_2O$** | -664.3490 | -664.5010 | -663.8189 | -663.6639 |
| **TBN-$H_2O$-$CO_2$** | -664.3695 | -664.5136 | -663.8338 | -663.6867 |
| **TBN-$H_2O$-$CO_2$'** | -664.3778 | -664.5283 | -663.8478 | -663.6944 |
| | | | | |
| **TBN*** | -399.3583 | -399.4855 | -399.0178 | -398.8876 |

| | | | | |
|---|---|---|---|---|
| **TBN*---$CO_2$** | -587.9374 | -588.0746 | -587.4486 | -587.3084 |
| **TS-TBN*** | -587.9337 | -588.0699 | -587.4423 | -587.3030 |
| **TBN*-$CO_2$** | -587.9445 | -588.0701 | -587.4451 | -587.3164 |
| | | | | |
| **MTBN** | -438.6384 | -438.7927 | -438.2718 | -438.1145 |
| **MTBN-H** | -439.1031 | -439.2121 | -438.6807 | -438.5687 |
| **MTBN---$CO_2$** | -627.2163 | -627.3779 | -626.6989 | -626.5343 |
| **TS-MTBN** | -627.2038 | -627.3648 | -626.6838 | -626.5199 |
| **MTBN-$CO_2$** | -627.2080 | -627.3577 | -626.6790 | -626.5264 |

**Notation:** $\boldsymbol{E_0^{DFT}}$ and $\boldsymbol{E_0^{CC}}$ refer to gas phase electronic energies calculated at the ωB97X-D/6-311G(d,p) and the LNO-CCSD(T)/CBS level. $\boldsymbol{G_0}$ is the Gibbs free energy calculated at the level of optimization, and $\boldsymbol{G}$ is the Gibbs free energy corrected with $\boldsymbol{E_0^{CC}}$ and concentration correction (0.001706). All values are in atomic units (Hartree).

**Table S8.** Electronic energies obtained from the LNO-CCSD(T) calculations. These values were used to approximate the LNO-CCSD(T)/CBS energies presented in Table S6.

| | $E_{TZ}^{HF}$ | $E_{TZ}^{C}(E_N)$ | $E_T$ | $E_{QZ}^{HF}$ | $E_{QZ}^{C}$ |
|---|---|---|---|---|---|
| | | | **MeCN** | | |
| **$CO_2$** | -187.7101 | -0.6301 | -0.6302 | -187.7230 | -0.6669 |
| **$H_2O$** | -76.0603 | -0.2821 | -0.2821 | -76.0657 | -0.2983 |
| | | | | | |
| **DBN** | -381.0881 | -1.7322 | -1.7322 | -381.1104 | -1.8066 |
| **DBN-H** | -381.5113 | -1.7175 | -1.7175 | -381.5338 | -1.7920 |
| **DBN---$CO_2$** | -568.8024 | -2.3677 | -2.3679 | -568.8373 | -2.4787 |
| **DBN-TS** | -568.7861 | -2.3766 | -2.3771 | -568.8207 | -2.4874 |
| **DBN-$CO_2$** | -568.7799 | -2.3766 | -2.3773 | -568.8142 | -2.4879 |
| | | | | | |
| **TBN** | -397.0954 | -1.7590 | -1.7591 | -397.1188 | -1.8368 |
| **TBN-H** | -397.5183 | -1.7424 | -1.7426 | -397.5420 | -1.8204 |
| **TBN---$CO_2$** | -584.8113 | -2.3938 | -2.3943 | -584.8474 | -2.5082 |
| **TS-TBN** | -584.7972 | -2.4006 | -2.4012 | -584.8331 | -2.5149 |
| **TBN-$CO_2$** | -584.8010 | -2.3984 | -2.3992 | -584.8366 | -2.5134 |
| | | | | | |
| **TBN-$H_2O$---$CO_2$** | -660.8782 | -2.6837 | -2.6842 | -660.9195 | -2.8139 |
| **TS-TBN-$H_2O$** | -660.8448 | -2.6956 | -2.6965 | -660.8856 | -2.8261 |
| **TBN-$H_2O$-$CO_2$** | -660.8719 | -2.6800 | -2.6810 | -660.9125 | -2.8112 |
| **TBN-$H_2O$-$CO_2$'** | -660.8873 | -2.6790 | -2.6799 | -660.9279 | -2.8103 |
| | | | | | |
| **TBN*** | -397.0948 | -1.7582 | -1.7584 | -397.1182 | -1.8360 |
| **TBN*---$CO_2$** | -584.8102 | -2.3938 | -2.3943 | -584.8463 | -2.5081 |

| | | | | | |
|---|---|---|---|---|---|
| **TS-TBN*** | -584.7976 | -2.4010 | -2.4016 | -584.8335 | -2.5153 |
| **TBN*-$CO_2$** | -584.7973 | -2.4011 | -2.4020 | -584.8328 | -2.5161 |
| | | | | | |
| **MTBN** | -436.1348 | -1.9566 | -1.9568 | -436.1605 | -2.0417 |
| **MTBN-H** | -436.5593 | -1.9407 | -1.9409 | -436.5852 | -2.0260 |
| **MTBN---$CO_2$** | -623.8467 | -2.5928 | -2.5930 | -623.8851 | -2.7144 |
| **TS-MTBN** | -623.8215 | -2.6042 | -2.6047 | -623.8595 | -2.7256 |
| **MTBN-$CO_2$** | -623.8172 | -2.6001 | -2.6008 | -623.8550 | -2.7221 |
| | | | | | |
| | | | **BuOAc** | | |
| | | | | | |
| **$CO_2$** | -187.7101 | -0.6300 | -0.6302 | -187.7230 | -0.6668 |
| **$H_2O$** | -76.0604 | -0.2820 | -0.2820 | -76.0658 | -0.2982 |
| | | | | | |
| **DBN** | -381.0884 | -1.7320 | -1.7321 | -381.1106 | -1.8065 |
| **DBN-H** | -381.5113 | -1.7175 | -1.7176 | -381.5338 | -1.7920 |
| **DBN---$CO_2$** | -568.8023 | -2.3678 | -2.3681 | -568.8372 | -2.4788 |
| **DBN-TS** | -568.7842 | -2.3775 | -2.3780 | -568.8188 | -2.4883 |
| **DBN-$CO_2$** | -568.7810 | -2.3769 | -2.3776 | -568.8153 | -2.4881 |
| | | | | | |
| **TBN** | -397.0957 | -1.7588 | -1.7589 | -397.1190 | -1.8366 |
| **TBN-H** | -397.5185 | -1.7422 | -1.7424 | -397.5422 | -1.8202 |
| **TBN---$CO_2$** | -584.8112 | -2.3939 | -2.3944 | -584.8473 | -2.5083 |
| **TS-TBN** | -584.7965 | -2.4007 | -2.4013 | -584.8324 | -2.5150 |
| **TBN-$CO_2$** | -584.8019 | -2.3986 | -2.3994 | -584.8375 | -2.5136 |
| | | | | | |
| **TBN-$H_2O$---$CO_2$** | -660.8793 | -2.6825 | -2.6832 | -660.9207 | -2.8129 |
| **TS-TBN-$H_2O$** | -660.8440 | -2.6959 | -2.6968 | -660.8847 | -2.8264 |
| **TBN-H2O-CO2** | -660.8726 | -2.6810 | -2.6821 | -660.9132 | -2.8122 |
| **TBN-$H_2O$-$CO_2$'** | -660.8876 | -2.6800 | -2.6809 | -660.9282 | -2.8113 |
| | | | | | |
| **TBN*** | -397.0951 | -1.7580 | -1.7582 | -397.1185 | -1.8359 |
| **TBN*---$CO_2$** | -584.8101 | -2.3940 | -2.3945 | -584.8462 | -2.5084 |
| **TS-TBN*** | -584.7963 | -2.4017 | -2.4024 | -584.8322 | -2.5160 |
| **TBN*-$CO_2$** | -584.7981 | -2.4013 | -2.4022 | -584.8337 | -2.5164 |
| | | | | | |
| **MTBN** | -436.1350 | -1.9563 | -1.9565 | -436.1607 | -2.0415 |
| **MTBN-H** | -436.5594 | -1.9406 | -1.9407 | -436.5854 | -2.0258 |
| **MTBN---$CO_2$** | -623.8467 | -2.5926 | -2.5928 | -623.8851 | -2.7142 |
| **TS-MTBN** | -623.8199 | -2.6045 | -2.6051 | -623.8579 | -2.7260 |
| **MTBN-$CO_2$** | -623.8183 | -2.6006 | -2.6012 | -623.8561 | -2.7226 |

**Notation:** $E_{TZ}^{HF}$ and $E_{TZ}^{C}$ $(E_N)$ refer to the Hartree Fock and correlation energy respectively with normal threshold and on TZ basis. $E_T$ is the correlation energy with tight threshold and the TZ basis set. $E_{QZ}^{HF}$ and $E_{QZ}^{C}$ refer to the Hartree Fock and correlation energy respectively with normal threshold and on TZ basis. For further details, see the Computational details section. All values are in atomic units (Hartree).

## 3.7 Cartesian coordinates

Cartesian coordinates of the optimized geometries are given below in standard XYZ format (coordinates are in Å). For each structure, the first line indicates total number of atoms, second line shows the notation of the molecule (as defined on Figures S1 to S5, with the additional '_mecn' or '_buoac' tags referring to the solvent in which it was optimized).

### 3.7.1 Reactants

```
3
CO2_buoac
C                0.00000      0.00000      0.00000
O                0.00000      0.00000      1.15605
O                0.00000      0.00000     -1.15605

3
CO2_mecn
C                0.00000      0.00000      0.00000
O                0.00000      0.00000      1.15621
O                0.00000      0.00000     -1.15621

3
H2O_buoac
O                0.00000      0.00000      0.11855
H                0.00000      0.75407     -0.47420
H                0.00000     -0.75407     -0.47420

3
H2O_mecn
O                0.00000      0.00000      0.11885
H                0.00000      0.75377     -0.47538
H                0.00000     -0.75377     -0.47538

21
DBN_buoac
C               -0.19795     -0.73518      0.03134
N               -0.22814      0.63282      0.01844
C               -1.62874     -1.22562      0.04590
C                0.97989      1.40610      0.19027
C               -1.56177      1.17535      0.18974
C                2.13533      0.60906     -0.40675
H                0.86153      2.36725     -0.31877
H                1.16208      1.61412      1.25466
C                2.12798     -0.82054      0.13807
H                2.02208      0.58505     -1.49554
H                3.08573      1.09928     -0.18211
N                0.83136     -1.49329      0.05765
H                2.86083     -1.42414     -0.40558
H                2.45491     -0.81380      1.18700
```

| | | | |
|---|---|---|---|
| H | -1.75730 | 1.42339 | 1.24345 |
| H | -1.68635 | 2.08705 | -0.40103 |
| C | -2.45083 | 0.02374 | -0.29312 |
| H | -3.43416 | 0.03232 | 0.17781 |
| H | -2.58779 | 0.09935 | -1.37477 |
| H | -1.77298 | -2.05641 | -0.64480 |
| H | -1.85458 | -1.58753 | 1.05433 |

21
DBN_mecn

| | | | |
|---|---|---|---|
| C | -0.19925 | -0.73459 | 0.03342 |
| N | -0.22725 | 0.62941 | 0.02995 |
| C | -1.63000 | -1.22488 | 0.04526 |
| C | 0.98165 | 1.40669 | 0.18704 |
| C | -1.56241 | 1.17576 | 0.19008 |
| C | 2.13448 | 0.60736 | -0.41072 |
| H | 0.85639 | 2.36275 | -0.32901 |
| H | 1.16906 | 1.62269 | 1.24817 |
| C | 2.12826 | -0.81873 | 0.14143 |
| H | 2.01923 | 0.57846 | -1.49937 |
| H | 3.08520 | 1.09805 | -0.18957 |
| N | 0.83205 | -1.49565 | 0.05378 |
| H | 2.86774 | -1.42249 | -0.39322 |
| H | 2.44751 | -0.80233 | 1.19260 |
| H | -1.76222 | 1.42620 | 1.24160 |
| H | -1.67871 | 2.08585 | -0.40412 |
| C | -2.45033 | 0.02505 | -0.29600 |
| H | -3.43430 | 0.03351 | 0.17320 |
| H | -2.58408 | 0.10058 | -1.37806 |
| H | -1.77525 | -2.05573 | -0.64565 |
| H | -1.85853 | -1.58388 | 1.05430 |

23
MTBN_buoac

| | | | |
|---|---|---|---|
| C | 0.25736 | 0.51755 | -0.09919 |
| N | 0.69984 | -0.79638 | -0.22655 |
| N | 1.17471 | 1.41668 | 0.01239 |
| C | -0.14405 | -1.89999 | 0.18668 |
| C | 2.10018 | -0.77621 | 0.17418 |
| C | -1.56315 | -1.63268 | -0.28680 |
| H | 0.24411 | -2.82279 | -0.25180 |
| H | -0.12359 | -2.01910 | 1.28300 |
| C | -2.02728 | -0.27378 | 0.21156 |
| H | -1.59131 | -1.65131 | -1.38019 |
| H | -2.23626 | -2.40829 | 0.08462 |
| N | -1.08395 | 0.77378 | -0.16414 |
| H | -2.99611 | -0.02072 | -0.22598 |
| H | -2.15795 | -0.29843 | 1.30500 |
| C | -1.52251 | 2.13390 | 0.07238 |
| H | 2.19806 | -1.03770 | 1.24001 |
| H | 2.69515 | -1.47772 | -0.41408 |
| C | 2.44933 | 0.69795 | -0.08066 |
| H | 3.17300 | 1.08587 | 0.63954 |
| H | 2.88019 | 0.82440 | -1.08295 |
| H | -2.51887 | 2.26405 | -0.35630 |
| H | -1.56588 | 2.37432 | 1.14409 |
| H | -0.83408 | 2.82841 | -0.40581 |

23
MTBN_mecn

| | | | |
|---|---|---|---|
| C | 0.25691 | 0.51677 | -0.10174 |

| | | | |
|---|---|---|---|
| N | 0.69958 | -0.79534 | -0.23102 |
| N | 1.17699 | 1.41692 | 0.01135 |
| C | -0.14568 | -1.89914 | 0.18656 |
| C | 2.09875 | -0.77650 | 0.17799 |
| C | -1.56515 | -1.63291 | -0.28495 |
| H | 0.24325 | -2.82237 | -0.24949 |
| H | -0.12256 | -2.01189 | 1.28256 |
| C | -2.02785 | -0.27318 | 0.21098 |
| H | -1.59804 | -1.65678 | -1.37835 |
| H | -2.23685 | -2.40653 | 0.09239 |
| N | -1.08282 | 0.77492 | -0.16915 |
| H | -2.99651 | -0.01882 | -0.22499 |
| H | -2.15303 | -0.29418 | 1.30425 |
| C | -1.52145 | 2.13471 | 0.07566 |
| H | 2.18818 | -1.03339 | 1.24507 |
| H | 2.69554 | -1.48161 | -0.40346 |
| C | 2.45199 | 0.69434 | -0.08080 |
| H | 3.17758 | 1.08120 | 0.63799 |
| H | 2.88325 | 0.81645 | -1.08363 |
| H | -2.53427 | 2.25296 | -0.31482 |
| H | -1.52733 | 2.38103 | 1.14667 |
| H | -0.86069 | 2.83395 | -0.43469 |

20
TBN_buoac

| | | | |
|---|---|---|---|
| C | -0.32933 | -0.72038 | -0.07056 |
| N | -0.31641 | 0.65780 | -0.23554 |
| N | -1.48457 | -1.27418 | 0.05355 |
| C | 0.84913 | 1.43201 | 0.14926 |
| C | -1.64836 | 1.10808 | 0.14652 |
| C | 2.10666 | 0.69308 | -0.28740 |
| H | 0.79279 | 2.41278 | -0.32971 |
| H | 0.86425 | 1.59618 | 1.23964 |
| C | 2.09690 | -0.72414 | 0.26715 |
| H | 2.14671 | 0.65800 | -1.38010 |
| H | 2.99226 | 1.22323 | 0.06922 |
| N | 0.85899 | -1.39136 | -0.12039 |
| H | 2.93375 | -1.29787 | -0.13517 |
| H | 2.20662 | -0.69305 | 1.36047 |
| H | 0.77835 | -2.36767 | 0.11943 |
| H | -1.65787 | 1.42562 | 1.20129 |
| H | -1.98264 | 1.94297 | -0.47267 |
| C | -2.45859 | -0.18242 | -0.06461 |
| H | -3.26356 | -0.29189 | 0.66554 |
| H | -2.91510 | -0.19163 | -1.06343 |

20
TBN_mecn

| | | | |
|---|---|---|---|
| C | -0.32825 | -0.72009 | -0.07018 |
| N | -0.31682 | 0.65591 | -0.23840 |
| N | -1.48652 | -1.27465 | 0.05288 |
| C | 0.84975 | 1.43132 | 0.14907 |
| C | -1.64796 | 1.10685 | 0.15007 |
| C | 2.10759 | 0.69392 | -0.28759 |
| H | 0.79119 | 2.41259 | -0.32782 |
| H | 0.86183 | 1.59070 | 1.23922 |
| C | 2.09811 | -0.72296 | 0.26617 |
| H | 2.15121 | 0.66150 | -1.38052 |
| H | 2.99175 | 1.22374 | 0.07234 |
| N | 0.85816 | -1.39242 | -0.12029 |
| H | 2.93371 | -1.29824 | -0.13567 |

| | | | |
|---|---|---|---|
| H | 2.20492 | -0.69260 | 1.35893 |
| H | 0.78133 | -2.36643 | 0.13215 |
| H | -1.65251 | 1.41701 | 1.20647 |
| H | -1.98216 | 1.94602 | -0.46274 |
| C | -2.45988 | -0.17967 | -0.06668 |
| H | -3.26785 | -0.28768 | 0.66028 |
| H | -2.91332 | -0.18471 | -1.06715 |

20
TBNa_buoac

| | | | |
|---|---|---|---|
| C | 0.21525 | -0.72312 | -0.02933 |
| N | 0.25115 | 0.65168 | 0.09240 |
| N | 1.52587 | -1.16215 | -0.11169 |
| C | -0.94674 | 1.40451 | -0.20362 |
| C | 1.58937 | 1.14191 | -0.17295 |
| C | -2.12365 | 0.62769 | 0.37735 |
| H | -0.86392 | 2.39383 | 0.25412 |
| H | -1.07023 | 1.54558 | -1.28860 |
| C | -2.11119 | -0.81788 | -0.12954 |
| H | -2.04085 | 0.63788 | 1.46896 |
| H | -3.06591 | 1.11276 | 0.11012 |
| N | -0.81095 | -1.48324 | -0.08052 |
| H | -2.82384 | -1.41064 | 0.45251 |
| H | -2.47511 | -0.83877 | -1.16636 |
| H | 1.72815 | 1.38064 | -1.23785 |
| H | 1.81457 | 2.03053 | 0.41992 |
| C | 2.42826 | -0.07121 | 0.23436 |
| H | 3.36545 | -0.13657 | -0.31925 |
| H | 2.64830 | -0.04181 | 1.30912 |
| H | 1.71317 | -2.08891 | 0.23835 |

20
TBN*_mecn

| | | | |
|---|---|---|---|
| C | 0.21728 | -0.72213 | -0.02924 |
| N | 0.25050 | 0.64952 | 0.08978 |
| N | 1.52738 | -1.16402 | -0.11219 |
| C | -0.94870 | 1.40439 | -0.20084 |
| C | 1.58949 | 1.14286 | -0.17407 |
| C | -2.12415 | 0.62617 | 0.37981 |
| H | -0.86304 | 2.39163 | 0.25986 |
| H | -1.07321 | 1.54812 | -1.28476 |
| C | -2.11175 | -0.81648 | -0.13289 |
| H | -2.04136 | 0.63280 | 1.47161 |
| H | -3.06658 | 1.11121 | 0.11404 |
| N | -0.81069 | -1.48510 | -0.08021 |
| H | -2.82874 | -1.41042 | 0.44276 |
| H | -2.47093 | -0.82994 | -1.17144 |
| H | 1.72578 | 1.38270 | -1.23852 |
| H | 1.81158 | 2.03128 | 0.41940 |
| C | 2.42900 | -0.06861 | 0.23319 |
| H | 3.36618 | -0.13373 | -0.31970 |
| H | 2.64765 | -0.04150 | 1.30763 |
| H | 1.71527 | -2.08218 | 0.26178 |

### 3.7.2 Precomplexes

24
DBN---$CO_2$_buoac

| | | | |
|---|---|---|---|
| C | 0.31876 | -0.33139 | -0.01639 |

| | | | |
|---|---|---|---|
| N | 1.41927 | 0.41354 | -0.07534 |
| C | 0.70157 | -1.77881 | 0.13125 |
| C | 1.43600 | 1.86940 | -0.05399 |
| C | 2.65295 | -0.36035 | 0.05130 |
| C | 0.08701 | 2.37626 | 0.42626 |
| H | 2.24100 | 2.18583 | 0.61335 |
| H | 1.66526 | 2.23816 | -1.05873 |
| C | -1.02522 | 1.62458 | -0.28516 |
| H | 0.00045 | 3.44529 | 0.22719 |
| H | -0.00452 | 2.22572 | 1.50585 |
| N | -0.89118 | 0.18030 | -0.07748 |
| H | -2.00810 | 1.90277 | 0.08373 |
| H | -1.00404 | 1.83196 | -1.36069 |
| H | 3.39507 | 0.00770 | -0.65956 |
| H | 3.05215 | -0.24071 | 1.06472 |
| C | 2.19066 | -1.78664 | -0.23570 |
| H | 2.75623 | -2.52558 | 0.33033 |
| H | 2.30754 | -2.00664 | -1.29899 |
| H | 0.52070 | -2.07066 | 1.16875 |
| H | 0.07939 | -2.42035 | -0.48400 |
| C | -2.20197 | -0.65834 | 0.01642 |
| O | -3.18903 | 0.02758 | -0.20449 |
| O | -2.01801 | -1.83491 | 0.29622 |

24

DBN---$CO_2$_mecn

| | | | |
|---|---|---|---|
| C | 0.43448 | -0.30570 | -0.13566 |
| N | 1.70809 | 0.18257 | -0.08265 |
| C | 0.50086 | -1.80188 | 0.06570 |
| C | 1.98869 | 1.60148 | 0.03866 |
| C | 2.70072 | -0.83573 | 0.21204 |
| C | 0.70326 | 2.34026 | 0.39759 |
| H | 2.74706 | 1.74548 | 0.81548 |
| H | 2.40496 | 1.98187 | -0.90205 |
| C | -0.45723 | 1.80884 | -0.44392 |
| H | 0.83711 | 3.41351 | 0.24435 |
| H | 0.47398 | 2.18045 | 1.45640 |
| N | -0.64140 | 0.36768 | -0.30686 |
| H | -1.38967 | 2.30019 | -0.15606 |
| H | -0.28376 | 2.05641 | -1.50122 |
| H | 3.61151 | -0.66937 | -0.36975 |
| H | 2.97024 | -0.81768 | 1.27795 |
| C | 1.97933 | -2.13182 | -0.17118 |
| H | 2.32784 | -2.98673 | 0.40869 |
| H | 2.14853 | -2.34471 | -1.22976 |
| H | 0.20283 | -2.02434 | 1.09541 |
| H | -0.18578 | -2.32508 | -0.59802 |
| C | -3.15169 | -0.45899 | 0.10035 |
| O | -3.54008 | 0.63206 | 0.11254 |
| O | -2.90018 | -1.58962 | 0.11292 |

26

MTBN---$CO_2$_buoac

| | | | |
|---|---|---|---|
| C | 0.42105 | 0.09722 | -0.39527 |
| N | 1.45028 | 1.01377 | -0.20732 |
| N | -0.74727 | 0.59571 | -0.61679 |
| C | 2.62545 | 0.65268 | 0.56069 |
| C | 0.79459 | 2.29102 | 0.04192 |
| C | 3.05133 | -0.75268 | 0.16934 |
| H | 3.41973 | 1.37244 | 0.34756 |
| H | 2.41508 | 0.70041 | 1.64222 |
| C | 1.88341 | -1.71174 | 0.33225 |
| H | 3.38492 | -0.75501 | -0.87244 |
| H | 3.88449 | -1.08079 | 0.79440 |
| N | 0.71057 | -1.23796 | -0.39465 |
| H | 2.14373 | -2.69668 | -0.06306 |
| H | 1.64690 | -1.83878 | 1.40043 |
| C | -0.39816 | -2.16537 | -0.48452 |
| H | 0.69098 | 2.46327 | 1.12496 |
| H | 1.35615 | 3.12043 | -0.39251 |
| C | -0.56849 | 2.04979 | -0.62470 |
| H | -1.38393 | 2.54805 | -0.09539 |
| H | -0.56667 | 2.42342 | -1.65719 |
| C | -3.22549 | -0.19184 | 0.45046 |
| O | -3.65470 | -0.55090 | -0.56198 |
| O | -2.88747 | 0.14597 | 1.50485 |
| H | -0.89742 | -2.30834 | 0.48488 |
| H | -1.13005 | -1.79171 | -1.19834 |
| H | -0.02378 | -3.13230 | -0.82818 |

26

MTBN---$CO_2$_mecn

| | | | |
|---|---|---|---|
| C | 0.42445 | 0.09824 | -0.45163 |
| N | 1.44382 | 1.01051 | -0.20343 |
| N | -0.73062 | 0.60322 | -0.73401 |
| C | 2.57236 | 0.64024 | 0.63140 |
| C | 0.77594 | 2.28592 | 0.02920 |
| C | 3.01712 | -0.76316 | 0.25678 |
| H | 3.37783 | 1.36080 | 0.47092 |
| H | 2.29534 | 0.68077 | 1.69725 |
| C | 1.83934 | -1.71859 | 0.34747 |
| H | 3.41305 | -0.76175 | -0.76323 |
| H | 3.81014 | -1.09731 | 0.92868 |
| N | 0.70878 | -1.23790 | -0.44417 |
| H | 2.11691 | -2.70321 | -0.03576 |
| H | 1.53913 | -1.84611 | 1.39872 |
| C | -0.40169 | -2.16117 | -0.57008 |
| H | 0.61164 | 2.43857 | 1.10723 |
| H | 1.36206 | 3.12141 | -0.35781 |
| C | -0.54614 | 2.05846 | -0.71667 |
| H | -1.38881 | 2.55501 | -0.23028 |
| H | -0.48250 | 2.44386 | -1.74320 |
| C | -3.18327 | -0.18719 | 0.52467 |
| O | -3.64551 | -0.62352 | -0.44183 |
| O | -2.79652 | 0.23327 | 1.53111 |
| H | -0.94076 | -2.28840 | 0.37975 |

| | | | |
|---|---|---|---|
| H | -1.10300 | -1.79521 | -1.31760 |
| H | -0.01727 | -3.13377 | -0.88443 |

23

TBN---$CO_2$_buoac

| | | | |
|---|---|---|---|
| C | 0.29911 | 0.03963 | -0.22625 |
| N | 1.40848 | 0.86856 | -0.17997 |
| N | -0.85014 | 0.62289 | -0.22757 |
| C | 2.66778 | 0.37983 | 0.35066 |
| C | 0.90433 | 2.17763 | 0.21569 |
| C | 2.90479 | -1.03757 | -0.15298 |
| H | 3.46961 | 1.04490 | 0.02040 |
| H | 2.65680 | 0.39508 | 1.45307 |
| C | 1.71008 | -1.91870 | 0.18344 |
| H | 3.05122 | -1.01801 | -1.23692 |
| H | 3.80682 | -1.44848 | 0.30510 |
| N | 0.49021 | -1.30585 | -0.32984 |
| H | 1.81835 | -2.90172 | -0.27823 |
| H | 1.65298 | -2.06404 | 1.27135 |
| H | -0.36142 | -1.83964 | -0.24288 |
| H | 1.00121 | 2.31212 | 1.30447 |
| H | 1.44448 | 2.98309 | -0.28564 |
| C | -0.56883 | 2.06149 | -0.21325 |
| H | -1.24318 | 2.58722 | 0.46598 |
| H | -0.71371 | 2.48418 | -1.21619 |
| C | -3.20490 | -0.61450 | 0.11342 |
| O | -3.80179 | 0.37416 | 0.16100 |
| O | -2.72285 | -1.66926 | 0.08610 |

23

TBN---$CO_2$_mecn

| | | | |
|---|---|---|---|
| C | 0.30844 | 0.03450 | -0.20233 |
| N | 1.41786 | 0.86334 | -0.19244 |
| N | -0.84212 | 0.61918 | -0.18331 |
| C | 2.68923 | 0.37859 | 0.31836 |
| C | 0.92320 | 2.17485 | 0.21116 |
| C | 2.91584 | -1.04332 | -0.17572 |
| H | 3.48308 | 1.04159 | -0.03365 |
| H | 2.69686 | 0.40424 | 1.41973 |
| C | 1.72844 | -1.91961 | 0.19493 |
| H | 3.04271 | -1.03627 | -1.26258 |
| H | 3.82583 | -1.44964 | 0.27001 |
| N | 0.49603 | -1.31188 | -0.30099 |
| H | 1.82512 | -2.90834 | -0.25632 |
| H | 1.69149 | -2.04941 | 1.28489 |
| H | -0.35066 | -1.84703 | -0.17680 |
| H | 1.04257 | 2.30956 | 1.29715 |
| H | 1.45380 | 2.97873 | -0.30214 |
| C | -0.55725 | 2.05905 | -0.18687 |
| H | -1.21558 | 2.59328 | 0.50159 |
| H | -0.72084 | 2.47491 | -1.19018 |
| C | -3.25065 | -0.60777 | 0.09653 |
| O | -3.82529 | 0.39522 | 0.11912 |

| | | | |
|---|---|---|---|
| O | -2.77724 | -1.66571 | 0.08702 |

23

TBN*--$CO_2$_buoac

| | | | |
|---|---|---|---|
| C | 0.40661 | -0.28748 | -0.15666 |
| N | 1.70057 | 0.08246 | 0.13645 |
| N | 0.38622 | -1.66281 | -0.28206 |
| C | 2.09312 | 1.46079 | -0.05226 |
| C | 2.59568 | -1.04414 | -0.04307 |
| C | 0.93030 | 2.33127 | 0.41409 |
| H | 2.99152 | 1.65592 | 0.53911 |
| H | 2.33396 | 1.66430 | -1.10688 |
| C | -0.36580 | 1.91105 | -0.28479 |
| H | 0.82102 | 2.21428 | 1.49711 |
| H | 1.14279 | 3.38409 | 0.21230 |
| N | -0.61262 | 0.47244 | -0.30825 |
| H | -1.21707 | 2.39560 | 0.20229 |
| H | -0.35537 | 2.28216 | -1.31905 |
| C | -3.10153 | -0.39166 | 0.08876 |
| H | 3.00360 | -1.07587 | -1.06398 |
| H | 3.42396 | -1.01288 | 0.66727 |
| C | 1.64245 | -2.21525 | 0.20839 |
| H | 1.92684 | -3.11195 | -0.34284 |
| H | 1.59871 | -2.45155 | 1.27911 |
| O | -3.53508 | 0.68061 | 0.07959 |
| O | -2.80362 | -1.51228 | 0.12443 |
| H | -0.48458 | -2.12292 | -0.06633 |

23

TBN*---$CO_2$_mecn

| | | | |
|---|---|---|---|
| C | 0.42263 | -0.29272 | -0.15705 |
| N | 1.70954 | 0.09281 | 0.13683 |
| N | 0.41785 | -1.66882 | -0.29354 |
| C | 2.08450 | 1.47797 | -0.04588 |
| C | 2.62123 | -1.02054 | -0.05302 |
| C | 0.91231 | 2.33061 | 0.42818 |
| H | 2.98235 | 1.68005 | 0.54324 |
| H | 2.31860 | 1.68836 | -1.10020 |
| C | -0.37847 | 1.89816 | -0.27210 |
| H | 0.80616 | 2.20665 | 1.51089 |
| H | 1.11069 | 3.38692 | 0.23124 |
| N | -0.60838 | 0.45506 | -0.30565 |
| H | -1.23551 | 2.36963 | 0.21825 |
| H | -0.37129 | 2.27702 | -1.30366 |
| C | -3.13787 | -0.40304 | 0.08978 |
| H | 3.02556 | -1.03707 | -1.07529 |
| H | 3.45087 | -0.98148 | 0.65466 |
| C | 1.68563 | -2.20536 | 0.19327 |
| H | 1.98159 | -3.09542 | -0.36195 |
| H | 1.64378 | -2.44677 | 1.26231 |
| O | -3.55860 | 0.67199 | 0.01468 |
| O | -2.83712 | -1.51837 | 0.18621 |
| H | -0.43990 | -2.14062 | -0.04925 |

26

TBN-$H_2O$---$CO_2$_buoac

| | | | |
|---|---|---|---|
| C | 0.94096 | 0.33832 | -0.07106 |
| N | 2.27248 | 0.01512 | -0.22608 |
| N | 0.66352 | 1.60413 | -0.07049 |
| C | 2.77688 | -1.26551 | 0.23262 |
| C | 3.01639 | 1.24607 | 0.00784 |
| C | 1.76486 | -2.34980 | -0.11587 |
| C | 0.39431 | -1.99276 | 0.44386 |
| N | 0.02139 | -0.65265 | 0.01459 |
| C | 1.93491 | 2.29853 | -0.29420 |
| H | 3.73343 | -1.46118 | -0.25798 |
| H | 2.95821 | -1.24539 | 1.31941 |
| H | 1.70093 | -2.44762 | -1.20347 |
| H | 2.09202 | -3.30779 | 0.29319 |
| H | -0.36043 | -2.69065 | 0.07754 |
| H | 0.41190 | -2.06358 | 1.54030 |
| H | -0.92091 | -0.32904 | 0.19305 |
| H | 3.35406 | 1.29747 | 1.05442 |
| H | 3.88783 | 1.31642 | -0.64569 |
| H | 2.02226 | 3.17881 | 0.34578 |
| H | 2.00527 | 2.63559 | -1.33651 |
| H | -1.12562 | 1.78499 | 0.13908 |
| O | -2.05354 | 1.55056 | 0.37235 |
| C | -3.93023 | -0.31075 | -0.22541 |
| O | -4.69542 | 0.24342 | 0.44073 |
| O | -3.21566 | -0.92053 | -0.90164 |
| H | -2.13220 | 1.79359 | 1.29660 |

26

TBN-$H_2O$---$CO_2$_mecn

| | | | |
|---|---|---|---|
| C | 0.57577 | 0.13832 | -0.40392 |
| N | 1.67136 | 0.88739 | -0.03821 |
| N | -0.54590 | 0.78196 | -0.49317 |
| C | 2.82689 | 0.25659 | 0.57798 |
| C | 1.14463 | 2.14290 | 0.48636 |
| C | 3.10039 | -1.06926 | -0.11846 |
| C | 1.84619 | -1.93061 | -0.11575 |
| N | 0.73326 | -1.17937 | -0.69270 |
| C | -0.23351 | 2.18452 | -0.19214 |
| H | 3.68286 | 0.92835 | 0.48231 |
| H | 2.64668 | 0.09402 | 1.65181 |
| H | 3.41559 | -0.88219 | -1.14940 |
| H | 3.90802 | -1.59577 | 0.39333 |
| H | 1.99584 | -2.82947 | -0.71550 |
| H | 1.61242 | -2.24369 | 0.91012 |
| H | -0.13808 | -1.67780 | -0.79816 |
| H | 1.05811 | 2.08929 | 1.58175 |
| H | 1.78633 | 2.98577 | 0.22491 |
| H | -0.99840 | 2.62907 | 0.44743 |
| H | -0.19112 | 2.77063 | -1.11929 |
| H | -2.05288 | 0.25806 | -1.38579 |

| | | | |
|---|---|---|---|
| O | -2.90692 | -0.04663 | -1.76355 |
| C | -2.64975 | -0.73981 | 0.98440 |
| O | -3.21162 | 0.23223 | 1.26241 |
| O | -2.11552 | -1.74580 | 0.77865 |
| H | -3.52764 | 0.62969 | -1.48585 |

### 3.7.3 Transition states

24
TS-DBN_buoac

| | | | |
|---|---|---|---|
| C | 0.34905 | -0.31218 | -0.04214 |
| N | 1.56699 | 0.27445 | -0.07095 |
| C | 0.54174 | -1.80938 | -0.01503 |
| C | 1.73434 | 1.70855 | -0.18211 |
| C | 2.66382 | -0.67359 | -0.18020 |
| C | 0.50152 | 2.38031 | 0.41068 |
| H | 2.63848 | 1.99610 | 0.36105 |
| H | 1.86883 | 1.99668 | -1.23269 |
| C | -0.76394 | 1.75853 | -0.17208 |
| H | 0.50699 | 2.24706 | 1.49701 |
| H | 0.52540 | 3.45249 | 0.20552 |
| N | -0.78280 | 0.30395 | -0.06320 |
| H | -1.64994 | 2.14010 | 0.33772 |
| H | -0.86419 | 2.03722 | -1.22896 |
| C | -2.64616 | -0.55428 | -0.00258 |
| H | 3.00361 | -0.75255 | -1.22120 |
| H | 3.50892 | -0.34754 | 0.43095 |
| C | 2.02979 | -1.97515 | 0.31777 |
| H | 2.47229 | -2.85641 | -0.14627 |
| H | 2.16204 | -2.05476 | 1.39942 |
| O | -3.33909 | 0.39432 | 0.08639 |
| O | -2.44768 | -1.71353 | -0.08075 |
| H | -0.12984 | -2.28877 | 0.69299 |
| H | 0.30133 | -2.20154 | -1.00750 |

24
TS-DBN_mecn

| | | | |
|---|---|---|---|
| C | 0.36132 | -0.31290 | -0.05317 |
| N | 1.57844 | 0.27224 | -0.10810 |
| C | 0.55211 | -1.79529 | 0.15861 |
| C | 1.76291 | 1.71341 | -0.06104 |
| C | 2.67710 | -0.65899 | 0.10664 |
| C | 0.46929 | 2.36966 | 0.40438 |
| H | 2.58223 | 1.93410 | 0.62891 |
| H | 2.05322 | 2.08097 | -1.05155 |
| C | -0.71845 | 1.74490 | -0.32208 |
| H | 0.51142 | 3.44453 | 0.21797 |
| H | 0.34923 | 2.21939 | 1.48210 |
| N | -0.77120 | 0.29842 | -0.14520 |
| H | -1.65815 | 2.16093 | 0.04495 |
| H | -0.66023 | 1.98014 | -1.39347 |
| H | 3.50819 | -0.42990 | -0.56440 |
| H | 3.03889 | -0.58479 | 1.14033 |

| | | | |
|---|---|---|---|
| C | 2.03093 | -2.01549 | -0.18241 |
| H | 2.48507 | -2.82056 | 0.39483 |
| H | 2.13512 | -2.25258 | -1.24396 |
| H | 0.34270 | -2.01928 | 1.20922 |
| H | -0.13501 | -2.38151 | -0.44692 |
| C | -2.69737 | -0.55053 | 0.03265 |
| O | -3.36143 | 0.41818 | -0.00860 |
| O | -2.49237 | -1.70501 | 0.11529 |

26
TS-MTBN_buoac

| | | | |
|---|---|---|---|
| C | 0.23047 | 0.07564 | -0.32098 |
| N | 1.00326 | 1.17949 | -0.07890 |
| N | -1.03323 | 0.34735 | -0.58314 |
| C | 2.28884 | 1.10067 | 0.58206 |
| C | 0.10556 | 2.31225 | 0.09809 |
| C | 2.99507 | -0.16341 | 0.11881 |
| H | 2.87100 | 1.98755 | 0.32170 |
| H | 2.15834 | 1.09321 | 1.67443 |
| C | 2.08568 | -1.36948 | 0.29813 |
| H | 3.26390 | -0.06275 | -0.93657 |
| H | 3.91342 | -0.30972 | 0.69031 |
| N | 0.77892 | -1.14763 | -0.31713 |
| H | 2.52739 | -2.24712 | -0.17767 |
| H | 1.95697 | -1.60166 | 1.36282 |
| C | 0.07040 | -2.31095 | -0.81623 |
| H | -0.10373 | 2.47720 | 1.16527 |
| H | 0.53485 | 3.22216 | -0.32419 |
| C | -1.12382 | 1.80950 | -0.66570 |
| H | -2.06566 | 2.15594 | -0.24305 |
| H | -1.08079 | 2.13171 | -1.71309 |
| C | -2.50578 | -0.47941 | 0.43441 |
| O | -3.42928 | 0.21709 | 0.18527 |
| O | -2.04229 | -1.40839 | 1.00490 |
| H | -0.25611 | -2.96093 | -0.00170 |
| H | -0.80505 | -1.98962 | -1.37591 |
| H | 0.73679 | -2.86883 | -1.48101 |

26
TS-MTBN_mecn

| | | | |
|---|---|---|---|
| C | 0.23738 | 0.08091 | -0.34450 |
| N | 1.00922 | 1.18172 | -0.08437 |
| N | -1.02378 | 0.35305 | -0.62046 |
| C | 2.28042 | 1.09005 | 0.60566 |
| C | 0.10649 | 2.30856 | 0.10839 |
| C | 2.99555 | -0.16602 | 0.13592 |
| H | 2.86751 | 1.98139 | 0.37453 |
| H | 2.12305 | 1.06208 | 1.69376 |
| C | 2.08546 | -1.37518 | 0.28353 |
| H | 3.28318 | -0.05010 | -0.91303 |
| H | 3.90324 | -0.32048 | 0.72181 |
| N | 0.78413 | -1.14378 | -0.34264 |
| H | 2.53237 | -2.24453 | -0.20216 |

| | | | |
|---|---|---|---|
| H | 1.94399 | -1.62341 | 1.34286 |
| C | 0.06530 | -2.30721 | -0.82597 |
| H | -0.11323 | 2.44798 | 1.17698 |
| H | 0.53664 | 3.22900 | -0.28886 |
| C | -1.11360 | 1.81803 | -0.67675 |
| H | -2.05869 | 2.16071 | -0.25665 |
| H | -1.05970 | 2.16185 | -1.71725 |
| C | -2.52345 | -0.48645 | 0.45925 |
| O | -3.44757 | 0.18720 | 0.16687 |
| O | -2.02750 | -1.37523 | 1.05823 |
| H | -0.26577 | -2.94375 | -0.00187 |
| H | -0.80714 | -1.98729 | -1.39174 |
| H | 0.72681 | -2.88236 | -1.48018 |

23
TS-TBN_buoac

| | | | |
|---|---|---|---|
| C | 0.21957 | -0.03347 | -0.11016 |
| N | 1.20138 | 0.92483 | -0.17125 |
| N | -0.99343 | 0.42855 | -0.05806 |
| C | 2.56375 | 0.61980 | 0.22398 |
| C | 0.56971 | 2.19031 | 0.18567 |
| C | 2.92194 | -0.77430 | -0.27526 |
| H | 3.22951 | 1.36762 | -0.21297 |
| H | 2.67058 | 0.67575 | 1.31853 |
| C | 1.89296 | -1.78924 | 0.20391 |
| H | 2.95095 | -0.77043 | -1.36869 |
| H | 3.91164 | -1.05535 | 0.08967 |
| N | 0.55262 | -1.34080 | -0.15431 |
| H | 2.06445 | -2.75805 | -0.26761 |
| H | 1.97930 | -1.92406 | 1.29001 |
| H | -0.22127 | -1.97632 | -0.02635 |
| H | 0.71792 | 2.40261 | 1.25473 |
| H | 0.97952 | 3.01647 | -0.39757 |
| C | -0.90322 | 1.88623 | -0.13616 |
| H | -1.59252 | 2.35836 | 0.56527 |
| H | -1.16223 | 2.22918 | -1.14539 |
| C | -2.77629 | -0.64524 | 0.03691 |
| O | -3.57331 | 0.21374 | 0.00641 |
| O | -2.39948 | -1.76104 | 0.09514 |

23
TS-TBN_mecn

| | | | |
|---|---|---|---|
| C | 0.23018 | -0.03234 | -0.18417 |
| N | 1.20946 | 0.93005 | -0.16982 |
| N | -0.98824 | 0.42219 | -0.18720 |
| C | 2.54799 | 0.61890 | 0.30230 |
| C | 0.55372 | 2.18098 | 0.19906 |
| C | 2.94201 | -0.76326 | -0.20109 |
| H | 3.23558 | 1.37834 | -0.07620 |
| H | 2.58314 | 0.65152 | 1.40175 |
| C | 1.88913 | -1.78860 | 0.19400 |
| H | 3.04150 | -0.73932 | -1.29034 |
| H | 3.90698 | -1.04856 | 0.22163 |

| | | | |
|---|---|---|---|
| N | 0.57137 | -1.33815 | -0.24634 |
| H | 2.09327 | -2.75001 | -0.27911 |
| H | 1.90239 | -1.93715 | 1.28104 |
| H | -0.20258 | -1.97903 | -0.14879 |
| H | 0.64786 | 2.35391 | 1.28087 |
| H | 0.98832 | 3.02868 | -0.33255 |
| C | -0.89846 | 1.88348 | -0.20749 |
| H | -1.62437 | 2.32837 | 0.47495 |
| H | -1.10692 | 2.26375 | -1.21534 |
| C | -2.79004 | -0.65121 | 0.08059 |
| O | -3.56567 | 0.22516 | 0.13352 |
| O | -2.41688 | -1.76726 | 0.09227 |

23
TS-TBN*_buoac

| | | | |
|---|---|---|---|
| C | 0.35134 | -0.30820 | -0.09410 |
| N | 1.60388 | 0.21125 | 0.07524 |
| N | 0.46133 | -1.66957 | -0.18714 |
| C | 1.83746 | 1.62691 | -0.10698 |
| C | 2.60805 | -0.81873 | -0.12302 |
| C | 0.61162 | 2.36819 | 0.41673 |
| H | 2.73340 | 1.90778 | 0.45211 |
| H | 2.01339 | 1.86257 | -1.16650 |
| C | -0.66074 | 1.81019 | -0.22057 |
| H | 0.56348 | 2.24741 | 1.50344 |
| H | 0.70038 | 3.43556 | 0.20217 |
| N | -0.75272 | 0.35597 | -0.16835 |
| H | -1.54177 | 2.21972 | 0.27852 |
| H | -0.71810 | 2.13428 | -1.26821 |
| C | -2.67050 | -0.50541 | 0.03362 |
| H | 2.96730 | -0.82898 | -1.16125 |
| H | 3.45850 | -0.67550 | 0.54533 |
| C | 1.80385 | -2.08086 | 0.20361 |
| H | 2.13531 | -2.94793 | -0.36734 |
| H | 1.86238 | -2.31169 | 1.27405 |
| O | -3.35011 | 0.44864 | -0.01149 |
| O | -2.43715 | -1.65616 | 0.13176 |
| H | -0.35001 | -2.21901 | 0.05158 |

23
TS-TBN*_mecn

| | | | |
|---|---|---|---|
| C | 0.35879 | -0.30902 | -0.07849 |
| N | 1.61674 | 0.19995 | 0.07250 |
| N | 0.45548 | -1.67485 | -0.17160 |
| C | 1.85891 | 1.61263 | -0.12721 |
| C | 2.61031 | -0.83868 | -0.14030 |
| C | 0.65017 | 2.36739 | 0.41523 |
| H | 2.76870 | 1.88958 | 0.41034 |
| H | 2.01367 | 1.83649 | -1.19222 |
| C | -0.63834 | 1.81649 | -0.19543 |
| H | 0.62184 | 2.25371 | 1.50358 |
| H | 0.74340 | 3.43248 | 0.19189 |
| N | -0.74276 | 0.36152 | -0.14207 |

| | | | |
|---|---|---|---|
| H | -1.50535 | 2.23566 | 0.32107 |
| H | -0.71229 | 2.14196 | -1.24178 |
| C | -2.71893 | -0.49505 | 0.02447 |
| H | 2.94818 | -0.85510 | -1.18534 |
| H | 3.47439 | -0.69834 | 0.51033 |
| C | 1.80268 | -2.09128 | 0.20746 |
| H | 2.12138 | -2.96604 | -0.35853 |
| H | 1.87093 | -2.31150 | 1.27914 |
| O | -3.36766 | 0.47773 | -0.03036 |
| O | -2.48807 | -1.64344 | 0.11769 |
| H | -0.34666 | -2.21449 | 0.11672 |

26

TS-TBN-$H_2O$_buoac

| | | | |
|---|---|---|---|
| C | 0.70462 | 0.18675 | -0.14196 |
| N | 2.00579 | 0.59325 | -0.04639 |
| N | -0.16708 | 1.15999 | -0.12563 |
| C | 3.05117 | -0.32546 | 0.36306 |
| C | 1.99281 | 1.98982 | 0.36950 |
| C | 2.78228 | -1.68519 | -0.26926 |
| C | 1.37142 | -2.15385 | 0.05992 |
| N | 0.40603 | -1.11455 | -0.27942 |
| C | 0.58636 | 2.41577 | -0.07911 |
| H | 4.01241 | 0.07151 | 0.02930 |
| H | 3.08460 | -0.40850 | 1.45981 |
| H | 2.89998 | -1.60818 | -1.35395 |
| H | 3.50569 | -2.41462 | 0.09946 |
| H | 1.12247 | -3.04768 | -0.51377 |
| H | 1.29967 | -2.40821 | 1.12490 |
| H | -0.58335 | -1.34181 | -0.25108 |
| H | 2.11459 | 2.06568 | 1.45947 |
| H | 2.79041 | 2.55504 | -0.11488 |
| H | 0.12714 | 3.12517 | 0.61115 |
| H | 0.61747 | 2.87806 | -1.07323 |
| H | -1.51461 | 1.02912 | -0.42652 |
| O | -2.59402 | 0.89002 | -0.66399 |
| C | -3.28672 | -0.54695 | 0.16614 |
| O | -4.32925 | -0.20672 | 0.61292 |
| O | -2.49035 | -1.42109 | 0.00750 |
| H | -3.09227 | 1.65053 | -0.35170 |

26

TS-TBN-$H_2O$_mecn

| | | | |
|---|---|---|---|
| C | 0.71244 | 0.18229 | -0.15633 |
| N | 2.00735 | 0.60638 | -0.05481 |
| N | -0.17585 | 1.14009 | -0.13946 |
| C | 3.06053 | -0.29815 | 0.37240 |
| C | 1.96890 | 1.99864 | 0.37825 |
| C | 2.81692 | -1.66527 | -0.25282 |
| C | 1.40865 | -2.14845 | 0.06372 |
| N | 0.43439 | -1.12524 | -0.30719 |
| C | 0.56053 | 2.40752 | -0.07673 |
| H | 4.01998 | 0.11014 | 0.04816 |

| | | | |
|---|---|---|---|
| H | 3.07908 | -0.37307 | 1.46953 |
| H | 2.94799 | -1.59726 | -1.33680 |
| H | 3.54397 | -2.38217 | 0.13251 |
| H | 1.17865 | -3.05400 | -0.49912 |
| H | 1.32572 | -2.38444 | 1.13173 |
| H | -0.54986 | -1.36577 | -0.26500 |
| H | 2.07992 | 2.06034 | 1.46991 |
| H | 2.76183 | 2.58196 | -0.09146 |
| H | 0.08577 | 3.10480 | 0.61511 |
| H | 0.59204 | 2.87840 | -1.06688 |
| H | -1.55078 | 1.00925 | -0.44707 |
| O | -2.61809 | 0.88895 | -0.67472 |
| C | -3.30051 | -0.56246 | 0.17512 |
| O | -4.33332 | -0.21934 | 0.64037 |
| O | -2.50471 | -1.42976 | -0.00644 |
| H | -3.09135 | 1.65968 | -0.34580 |

### 3.7.4 Products

24

DBN-$CO_2$_buoac

| | | | |
|---|---|---|---|
| C | -0.31691 | -0.33041 | 0.03303 |
| N | -1.42212 | 0.40818 | 0.09470 |
| C | -0.69238 | -1.78708 | -0.01452 |
| C | -1.43048 | 1.85911 | 0.17517 |
| C | -2.64562 | -0.38410 | 0.19928 |
| C | -0.13871 | 2.37877 | -0.43180 |
| H | -2.30342 | 2.22230 | -0.37091 |
| H | -1.53056 | 2.16837 | 1.22131 |
| C | 1.04551 | 1.64070 | 0.16645 |
| H | -0.15775 | 2.23158 | -1.51557 |
| H | -0.04025 | 3.44807 | -0.23956 |
| N | 0.89216 | 0.18669 | 0.04287 |
| H | 1.97619 | 1.89663 | -0.33211 |
| H | 1.15985 | 1.89078 | 1.22660 |
| C | 2.20560 | -0.65843 | 0.01092 |
| H | -2.98453 | -0.39931 | 1.24101 |
| H | -3.42901 | 0.06454 | -0.41384 |
| C | -2.20000 | -1.75853 | -0.29420 |
| H | -2.73102 | -2.56888 | 0.20346 |
| H | -2.37879 | -1.84005 | -1.36843 |
| O | 3.19568 | 0.05567 | -0.04094 |
| O | 2.01966 | -1.86633 | 0.05543 |
| H | -0.10557 | -2.32469 | -0.75209 |
| H | -0.45033 | -2.22828 | 0.95533 |

24

DBN-$CO_2$_mecn

| | | | |
|---|---|---|---|
| C | -0.31866 | -0.33306 | 0.03181 |
| N | -1.41195 | 0.41268 | 0.10125 |
| C | -0.70475 | -1.78642 | -0.01922 |
| C | -1.41313 | 1.86457 | 0.18411 |
| C | -2.64507 | -0.36834 | 0.19955 |

| | | | |
|---|---|---|---|
| C | -0.12524 | 2.37716 | -0.43347 |
| H | -2.28971 | 2.22932 | -0.35367 |
| H | -1.50194 | 2.16885 | 1.23200 |
| C | 1.05953 | 1.63582 | 0.15776 |
| H | -0.15347 | 2.22885 | -1.51684 |
| H | -0.01951 | 3.44545 | -0.24064 |
| N | 0.89966 | 0.17972 | 0.03598 |
| H | 1.98527 | 1.89055 | -0.34961 |
| H | 1.17853 | 1.88616 | 1.21703 |
| C | 2.18149 | -0.65878 | 0.01299 |
| H | -2.98288 | -0.38115 | 1.24091 |
| H | -3.41969 | 0.09340 | -0.41403 |
| C | -2.21215 | -1.74461 | -0.29747 |
| H | -2.74854 | -2.55092 | 0.20071 |
| H | -2.39170 | -1.82159 | -1.37180 |
| O | 3.19244 | 0.03562 | -0.03970 |
| O | 2.00646 | -1.87286 | 0.06338 |
| H | -0.12552 | -2.32580 | -0.76147 |
| H | -0.46820 | -2.22997 | 0.95103 |

26

MTBN-$CO_2$_buoac

| | | | |
|---|---|---|---|
| C | 0.18693 | 0.03815 | -0.14929 |
| N | 0.92291 | 1.15028 | 0.03179 |
| N | -1.11280 | 0.32791 | -0.36453 |
| C | 2.33193 | 1.16871 | 0.36965 |
| C | 0.05417 | 2.31774 | 0.11429 |
| C | 2.97119 | -0.13413 | -0.08483 |
| H | 2.79650 | 2.02425 | -0.12551 |
| H | 2.44656 | 1.30153 | 1.45247 |
| C | 2.11026 | -1.31246 | 0.34400 |
| H | 3.07237 | -0.13882 | -1.17363 |
| H | 3.96830 | -0.22554 | 0.34838 |
| N | 0.74280 | -1.16629 | -0.16302 |
| H | 2.50866 | -2.24351 | -0.05796 |
| H | 2.08540 | -1.40349 | 1.43506 |
| C | 0.09068 | -2.34618 | -0.71054 |
| H | -0.10006 | 2.60867 | 1.16023 |
| H | 0.49290 | 3.15541 | -0.42878 |
| C | -1.21676 | 1.78307 | -0.54742 |
| H | -2.13506 | 2.13666 | -0.08866 |
| H | -1.23817 | 2.02579 | -1.61376 |
| C | -2.30644 | -0.41497 | 0.26852 |
| O | -3.36325 | 0.16393 | 0.04979 |
| O | -1.99800 | -1.42659 | 0.88898 |
| H | -0.23554 | -3.01827 | 0.08230 |
| H | -0.78023 | -2.05359 | -1.29065 |
| H | 0.80630 | -2.85071 | -1.36550 |

26

MTBN-$CO_2$_mecn

| | | | |
|---|---|---|---|
| C | 0.18714 | 0.03431 | -0.12621 |
| N | 0.91659 | 1.14246 | 0.06175 |
| N | -1.11806 | 0.32872 | -0.34932 |
| C | 2.33867 | 1.16857 | 0.34880 |

| | | | |
|---|---|---|---|
| C | 0.05514 | 2.31723 | 0.12149 |
| C | 2.96611 | -0.13653 | -0.11428 |
| H | 2.77928 | 2.02138 | -0.17134 |
| H | 2.48679 | 1.31235 | 1.42512 |
| C | 2.11618 | -1.31173 | 0.34278 |
| H | 3.04080 | -0.14882 | -1.20510 |
| H | 3.97246 | -0.22533 | 0.29688 |
| N | 0.73817 | -1.17046 | -0.14238 |
| H | 2.50692 | -2.24690 | -0.05569 |
| H | 2.10863 | -1.38706 | 1.43490 |
| C | 0.08958 | -2.34410 | -0.70749 |
| H | -0.10019 | 2.62508 | 1.16152 |
| H | 0.50431 | 3.14115 | -0.43297 |
| C | -1.21724 | 1.78544 | -0.53891 |
| H | -2.13111 | 2.14756 | -0.07820 |
| H | -1.23748 | 2.02425 | -1.60569 |
| C | -2.29176 | -0.40428 | 0.25628 |
| O | -3.36573 | 0.14224 | 0.00413 |
| O | -2.00229 | -1.40567 | 0.91130 |
| H | -0.23424 | -3.02844 | 0.07630 |
| H | -0.77929 | -2.04652 | -1.28869 |
| H | 0.80748 | -2.83975 | -1.36562 |

23

TBN-$CO_2$_buoac

| | | | |
|---|---|---|---|
| C | 0.17151 | -0.09428 | 0.01044 |
| N | 0.99531 | 0.96214 | -0.05749 |
| N | -1.11315 | 0.27897 | 0.03611 |
| C | 2.42564 | 0.82526 | 0.14763 |
| C | 0.23693 | 2.18914 | 0.16636 |
| C | 2.86892 | -0.52862 | -0.39878 |
| H | 2.92718 | 1.63697 | -0.38235 |
| H | 2.66493 | 0.91607 | 1.21507 |
| C | 2.02030 | -1.65581 | 0.17975 |
| H | 2.77627 | -0.52374 | -1.48826 |
| H | 3.91760 | -0.69819 | -0.15050 |
| N | 0.60376 | -1.34015 | 0.03840 |
| H | 2.21203 | -2.58930 | -0.34952 |
| H | 2.25794 | -1.81062 | 1.23749 |
| H | -0.15213 | -2.02649 | 0.08890 |
| H | 0.36320 | 2.52694 | 1.20152 |
| H | 0.57031 | 2.97779 | -0.50846 |
| C | -1.20203 | 1.73142 | -0.11818 |
| H | -1.92559 | 2.14451 | 0.58079 |
| H | -1.51419 | 1.98141 | -1.13551 |
| C | -2.29158 | -0.62529 | -0.00784 |
| O | -3.35707 | -0.02975 | -0.10029 |
| O | -2.00257 | -1.83188 | 0.06220 |

23

TBN-$CO_2$_mecn

| | | | |
|---|---|---|---|
| C | 0.17378 | -0.09846 | 0.01807 |
| N | 0.98969 | 0.95848 | -0.04873 |

| | | | |
|---|---|---|---|
| N | -1.11759 | 0.27385 | 0.04221 |
| C | 2.42504 | 0.83082 | 0.13734 |
| C | 0.23093 | 2.18715 | 0.16520 |
| C | 2.86922 | -0.52281 | -0.40674 |
| H | 2.91187 | 1.64379 | -0.40355 |
| H | 2.67379 | 0.92868 | 1.20101 |
| C | 2.03084 | -1.64977 | 0.18501 |
| H | 2.76872 | -0.52465 | -1.49560 |
| H | 3.91981 | -0.68638 | -0.16365 |
| N | 0.61018 | -1.34214 | 0.04735 |
| H | 2.22281 | -2.58683 | -0.33720 |
| H | 2.27211 | -1.79198 | 1.24311 |
| H | -0.13273 | -2.03878 | 0.09743 |
| H | 0.35958 | 2.53201 | 1.19687 |
| H | 0.56391 | 2.96878 | -0.51727 |
| C | -1.20736 | 1.72796 | -0.11425 |
| H | -1.92583 | 2.14365 | 0.58839 |
| H | -1.52092 | 1.97614 | -1.13145 |
| C | -2.28264 | -0.62053 | -0.01076 |
| O | -3.35748 | -0.03180 | -0.10495 |
| O | -2.00852 | -1.83343 | 0.05407 |

23

TBN*-$CO_2$_buoac

| | | | |
|---|---|---|---|
| C | 0.32468 | -0.33580 | -0.03753 |
| N | 1.46103 | 0.38060 | 0.02662 |
| N | 0.59850 | -1.64183 | -0.08504 |
| C | 1.50032 | 1.82174 | -0.11877 |
| C | 2.61172 | -0.49562 | -0.16647 |
| C | 0.19182 | 2.38367 | 0.41738 |
| H | 2.35345 | 2.19939 | 0.44852 |
| H | 1.64391 | 2.09308 | -1.17242 |
| C | -0.99402 | 1.66500 | -0.20813 |
| H | 0.16372 | 2.26549 | 1.50440 |
| H | 0.12816 | 3.44973 | 0.19318 |
| N | -0.88678 | 0.20997 | -0.05236 |
| H | -1.92957 | 1.95951 | 0.25962 |
| H | -1.06835 | 1.90500 | -1.27436 |
| C | -2.16266 | -0.61330 | 0.00393 |
| H | 2.96212 | -0.43961 | -1.20370 |
| H | 3.42628 | -0.21623 | 0.50171 |
| C | 2.01620 | -1.87146 | 0.16275 |
| H | 2.40485 | -2.66001 | -0.47959 |
| H | 2.18802 | -2.14151 | 1.20943 |
| O | -3.17381 | 0.06784 | -0.07835 |
| O | -1.98001 | -1.83108 | 0.12692 |
| H | -0.17959 | -2.27554 | 0.08118 |

23

TBN*-$CO_2$_mecn

| | | | |
|---|---|---|---|
| C | 0.32682 | -0.33878 | -0.03477 |
| N | 1.45414 | 0.38402 | 0.02155 |
| N | 0.60666 | -1.64367 | -0.08891 |

| | | | |
|---|---|---|---|
| C | 1.49007 | 1.82728 | -0.11302 |
| C | 2.61288 | -0.48352 | -0.17325 |
| C | 0.18037 | 2.38163 | 0.42435 |
| H | 2.34190 | 2.20040 | 0.45826 |
| H | 1.63417 | 2.10306 | -1.16462 |
| C | -1.00083 | 1.66075 | -0.20581 |
| H | 0.15070 | 2.25981 | 1.51095 |
| H | 0.11174 | 3.44747 | 0.20155 |
| N | -0.89211 | 0.20427 | -0.04300 |
| H | -1.93709 | 1.95824 | 0.25803 |
| H | -1.06650 | 1.89638 | -1.27327 |
| C | -2.14893 | -0.61280 | 0.00418 |
| H | 2.95942 | -0.41997 | -1.21064 |
| H | 3.42410 | -0.19666 | 0.49504 |
| C | 2.02930 | -1.86353 | 0.15376 |
| H | 2.42060 | -2.64707 | -0.49248 |
| H | 2.20359 | -2.13491 | 1.19912 |
| O | -3.17206 | 0.05475 | -0.11000 |
| O | -1.97871 | -1.83208 | 0.15449 |
| H | -0.15546 | -2.28665 | 0.10209 |

26

TBN-$H_2O$-$CO_2$_buoac

| | | | |
|---|---|---|---|
| C | -0.73681 | 0.20539 | -0.07514 |
| N | -2.05700 | 0.42579 | 0.04061 |
| N | -0.06527 | 1.35884 | -0.20758 |
| C | -3.01699 | -0.65514 | -0.08591 |
| C | -2.34289 | 1.83339 | -0.21379 |
| C | -2.39736 | -1.91607 | 0.50896 |
| C | -1.02567 | -2.18823 | -0.09868 |
| N | -0.19350 | -0.98918 | -0.06215 |
| C | -0.97288 | 2.47633 | 0.04588 |
| H | -3.92165 | -0.37590 | 0.45723 |
| H | -3.28412 | -0.80648 | -1.13965 |
| H | -2.30104 | -1.79053 | 1.59103 |
| H | -3.05258 | -2.76906 | 0.32603 |
| H | -0.50921 | -2.97050 | 0.45835 |
| H | -1.12772 | -2.52749 | -1.13509 |
| H | 0.85277 | -1.05331 | -0.18135 |
| H | -2.66876 | 1.97556 | -1.25099 |
| H | -3.11734 | 2.20231 | 0.45878 |
| H | -0.76900 | 3.30854 | -0.62605 |
| H | -0.88696 | 2.81983 | 1.08172 |
| H | 0.93134 | 1.38065 | 0.02179 |
| O | 2.61925 | 0.88274 | 0.56005 |
| C | 3.24918 | -0.24735 | -0.03523 |
| O | 4.47153 | -0.21655 | -0.06771 |
| O | 2.43278 | -1.10140 | -0.43589 |
| H | 3.33669 | 1.47003 | 0.81380 |

26

TBN-$H_2O$-$CO_2$_mecn

| | | | |
|---|---|---|---|
| C | -0.74487 | 0.20778 | -0.09091 |

| | | | |
|---|---|---|---|
| N | -2.06073 | 0.41942 | 0.03535 |
| N | -0.07751 | 1.36498 | -0.23782 |
| C | -3.01968 | -0.66671 | -0.06407 |
| C | -2.35955 | 1.82727 | -0.20896 |
| C | -2.38393 | -1.92131 | 0.52575 |
| C | -1.02238 | -2.18982 | -0.10474 |
| N | -0.19365 | -0.98618 | -0.07680 |
| C | -0.99103 | 2.47713 | 0.03484 |
| H | -3.91307 | -0.38514 | 0.49546 |
| H | -3.30521 | -0.82368 | -1.11130 |
| H | -2.26941 | -1.79167 | 1.60563 |
| H | -3.03767 | -2.77780 | 0.35558 |
| H | -0.49492 | -2.97172 | 0.44226 |
| H | -1.14241 | -2.52389 | -1.14059 |
| H | 0.84211 | -1.04760 | -0.20917 |
| H | -2.70064 | 1.96863 | -1.24067 |
| H | -3.12672 | 2.18668 | 0.47625 |
| H | -0.80158 | 3.31373 | -0.63528 |
| H | -0.89140 | 2.81313 | 1.07135 |
| H | 0.90987 | 1.39334 | 0.01875 |
| O | 2.60765 | 0.84167 | 0.61348 |
| C | 3.26091 | -0.23256 | -0.03204 |
| O | 4.48705 | -0.18105 | -0.05835 |
| O | 2.46988 | -1.08475 | -0.48506 |
| H | 3.30077 | 1.44081 | 0.90669 |

26

TBN-$H_2O$-$CO_2$'_buoac

| | | | |
|---|---|---|---|
| C | 0.73284 | 0.19294 | 0.04991 |
| N | 2.04408 | 0.47704 | -0.07519 |
| N | 0.00028 | 1.30165 | 0.14347 |
| C | 3.05830 | -0.54506 | 0.10058 |
| C | 2.25132 | 1.90144 | 0.16170 |
| C | 2.51344 | -1.86013 | -0.44824 |
| C | 1.15470 | -2.18395 | 0.16348 |
| N | 0.25929 | -1.03568 | 0.07228 |
| C | 0.84710 | 2.46423 | -0.10676 |
| H | 3.95283 | -0.24038 | -0.44599 |
| H | 3.32425 | -0.64218 | 1.16162 |
| H | 2.41649 | -1.78090 | -1.53467 |
| H | 3.21358 | -2.66818 | -0.23034 |
| H | 0.68759 | -3.01620 | -0.36407 |
| H | 1.27026 | -2.47616 | 1.21313 |
| H | -0.77953 | -1.14847 | 0.14822 |
| H | 2.56784 | 2.07454 | 1.19767 |
| H | 3.00580 | 2.30418 | -0.51439 |
| H | 0.59312 | 3.28709 | 0.56006 |
| H | 0.74687 | 2.80143 | -1.14368 |
| H | -1.03456 | 1.26631 | -0.00186 |
| O | -2.66223 | 0.99604 | -0.22023 |
| C | -3.07646 | -0.16728 | -0.00892 |
| O | -4.43503 | -0.33549 | -0.04314 |

| | | | |
|---|---|---|---|
| O | -2.42547 | -1.19949 | 0.22946 |
| H | -4.79554 | 0.53624 | -0.22889 |

26
TBN-$H_2O$-$CO_2$'_mecn

| | | | |
|---|---|---|---|
| C | 0.74437 | 0.19324 | 0.06382 |
| N | 2.05065 | 0.47287 | -0.07027 |
| N | 0.01309 | 1.30548 | 0.17462 |
| C | 3.06643 | -0.55355 | 0.08077 |
| C | 2.26635 | 1.89792 | 0.16205 |
| C | 2.51009 | -1.86289 | -0.46890 |
| C | 1.15984 | -2.18744 | 0.15993 |
| N | 0.26531 | -1.03509 | 0.08147 |
| C | 0.86288 | 2.46535 | -0.09386 |
| H | 3.95134 | -0.24437 | -0.47790 |
| H | 3.34651 | -0.65730 | 1.13659 |
| H | 2.39868 | -1.77793 | -1.55358 |
| H | 3.21038 | -2.67375 | -0.26349 |
| H | 0.68438 | -3.01732 | -0.36361 |
| H | 1.28956 | -2.47880 | 1.20766 |
| H | -0.76511 | -1.14578 | 0.17621 |
| H | 2.59330 | 2.06863 | 1.19444 |
| H | 3.01564 | 2.29513 | -0.52226 |
| H | 0.62078 | 3.29304 | 0.57089 |
| H | 0.75189 | 2.79406 | -1.13204 |
| H | -1.01001 | 1.27262 | -0.00383 |
| O | -2.67087 | 0.98558 | -0.27584 |
| C | -3.09522 | -0.16145 | -0.01159 |
| O | -4.45665 | -0.32677 | -0.05354 |
| O | -2.45485 | -1.18521 | 0.28726 |
| H | -4.82018 | 0.53314 | -0.28611 |

### 3.7.5 Protonated bases

22
DBN-H_buoac

| | | | |
|---|---|---|---|
| C | -0.24222 | 0.67520 | -0.04441 |
| N | -0.25633 | -0.63768 | -0.08924 |
| C | -1.62989 | 1.23248 | -0.03245 |
| C | 0.95649 | -1.44231 | -0.17870 |
| C | -1.61393 | -1.18668 | -0.16683 |
| C | 2.11819 | -0.66190 | 0.42535 |
| H | 0.78389 | -2.37084 | 0.36679 |
| H | 1.14305 | -1.69026 | -1.22803 |
| C | 2.18586 | 0.74597 | -0.15150 |
| H | 1.99410 | -0.60610 | 1.50992 |
| H | 3.05259 | -1.18442 | 0.22010 |
| N | 0.86863 | 1.37742 | -0.04688 |
| H | 2.89712 | 1.35913 | 0.40030 |
| H | 2.48909 | 0.72571 | -1.20184 |
| H | -1.81924 | -1.49672 | -1.19565 |
| H | -1.69516 | -2.05595 | 0.48610 |
| C | -2.48275 | -0.00657 | 0.28260 |

| | | | |
|---|---|---|---|
| H | -3.44463 | 0.01126 | -0.22619 |
| H | -2.66179 | -0.06852 | 1.35713 |
| H | -1.73510 | 2.04184 | 0.68994 |
| H | -1.83957 | 1.63663 | -1.02759 |
| H | 0.79905 | 2.38290 | -0.00252 |

22
DBN-H_mecn

| | | | |
|---|---|---|---|
| C | -0.24187 | 0.67514 | -0.04491 |
| N | -0.25628 | -0.63821 | -0.08795 |
| C | -1.62885 | 1.23195 | -0.03448 |
| C | 0.95580 | -1.44238 | -0.18025 |
| C | -1.61324 | -1.18618 | -0.16685 |
| C | 2.11666 | -0.66226 | 0.42553 |
| H | 0.78288 | -2.37204 | 0.36312 |
| H | 1.14304 | -1.68564 | -1.23044 |
| C | 2.18419 | 0.74598 | -0.15042 |
| H | 1.99004 | -0.60681 | 1.50998 |
| H | 3.05134 | -1.18414 | 0.21963 |
| N | 0.86789 | 1.37761 | -0.04615 |
| H | 2.89497 | 1.35933 | 0.40167 |
| H | 2.48702 | 0.72391 | -1.20081 |
| H | -1.81918 | -1.49242 | -1.19672 |
| H | -1.69427 | -2.05698 | 0.48411 |
| C | -2.48082 | -0.00617 | 0.28492 |
| H | -3.44412 | 0.01096 | -0.22161 |
| H | -2.65396 | -0.06737 | 1.36062 |
| H | -1.73081 | 2.04504 | 0.68398 |
| H | -1.83639 | 1.63030 | -1.03231 |
| H | 0.79691 | 2.38357 | -0.00376 |

21
TBN-H_buoac

| | | | |
|---|---|---|---|
| C | -0.26728 | -0.67285 | 0.01695 |
| N | -0.27310 | 0.65815 | -0.01738 |
| N | -1.51351 | -1.16304 | 0.05054 |
| C | 0.93287 | 1.45046 | 0.16580 |
| C | -1.63595 | 1.15922 | 0.15307 |
| C | 2.11629 | 0.66828 | -0.39109 |
| H | 0.80295 | 2.39101 | -0.37095 |
| H | 1.07083 | 1.67760 | 1.22904 |
| C | 2.15759 | -0.74079 | 0.18500 |
| H | 2.03780 | 0.61761 | -1.48018 |
| H | 3.04429 | 1.18471 | -0.14385 |
| N | 0.84900 | -1.38262 | 0.02740 |
| H | 2.89167 | -1.35009 | -0.34085 |
| H | 2.42329 | -0.71858 | 1.24593 |
| H | 0.78184 | -2.38714 | 0.08532 |
| H | -1.78702 | 1.48639 | 1.18669 |
| H | -1.82649 | 1.99367 | -0.52058 |
| C | -2.47474 | -0.08111 | -0.18629 |
| H | -3.34355 | -0.18672 | 0.46008 |
| H | -2.79454 | -0.07628 | -1.23136 |

| | | | |
|---|---|---|---|
| H | -1.71050 | -2.11899 | -0.20376 |

21
TBN-H_mecn

| | | | |
|---|---|---|---|
| C | -0.26732 | -0.67199 | 0.01694 |
| N | -0.27347 | 0.65957 | -0.02507 |
| N | -1.51406 | -1.16289 | 0.06184 |
| C | 0.93192 | 1.44992 | 0.16686 |
| C | -1.63552 | 1.15810 | 0.15628 |
| C | 2.11623 | 0.66857 | -0.38925 |
| H | 0.80432 | 2.39314 | -0.36573 |
| H | 1.06664 | 1.66976 | 1.23199 |
| C | 2.15551 | -0.74154 | 0.18444 |
| H | 2.03888 | 0.61974 | -1.47869 |
| H | 3.04373 | 1.18405 | -0.13790 |
| N | 0.84771 | -1.38236 | 0.02403 |
| H | 2.89008 | -1.35091 | -0.34053 |
| H | 2.41875 | -0.71906 | 1.24595 |
| H | 0.77684 | -2.38727 | 0.08359 |
| H | -1.78245 | 1.47339 | 1.19437 |
| H | -1.82989 | 1.99871 | -0.50836 |
| C | -2.47085 | -0.08064 | -0.19173 |
| H | -3.34966 | -0.18322 | 0.44136 |
| H | -2.77369 | -0.07704 | -1.24199 |
| H | -1.70459 | -2.11599 | -0.21096 |

24
MTBN-H_buoac

| | | | |
|---|---|---|---|
| C | 0.21407 | 0.44484 | -0.02134 |
| N | 0.63108 | -0.82518 | -0.03574 |
| N | 1.25563 | 1.28999 | 0.02513 |
| C | -0.26823 | -1.94349 | 0.18803 |
| C | 2.07549 | -0.87969 | 0.17876 |
| C | -1.63237 | -1.57445 | -0.37564 |
| H | 0.14084 | -2.81582 | -0.32324 |
| H | -0.32695 | -2.16836 | 1.25951 |
| C | -2.09566 | -0.22768 | 0.15836 |
| H | -1.57637 | -1.53663 | -1.46664 |
| H | -2.36323 | -2.33605 | -0.10204 |
| N | -1.06097 | 0.80005 | -0.02899 |
| H | -2.98446 | 0.10372 | -0.37884 |
| H | -2.34346 | -0.29219 | 1.22326 |
| C | -1.43076 | 2.20643 | 0.06474 |
| H | 2.28960 | -1.11888 | 1.22584 |
| H | 2.53260 | -1.63166 | -0.46327 |
| C | 2.50266 | 0.54756 | -0.18276 |
| H | 3.29117 | 0.92613 | 0.46427 |
| H | 2.81980 | 0.61937 | -1.22637 |
| H | -2.50982 | 2.28532 | -0.05171 |
| H | -1.14782 | 2.62925 | 1.03307 |
| H | -0.96438 | 2.78170 | -0.73785 |
| H | 1.17110 | 2.25895 | -0.23973 |

24
MTBN-H_mecn

| | | | |
|---|---|---|---|
| C | 0.21464 | 0.44551 | -0.02473 |
| N | 0.63231 | -0.82502 | -0.04680 |
| N | 1.25572 | 1.29116 | 0.03399 |
| C | -0.26571 | -1.94156 | 0.18955 |
| C | 2.07478 | -0.87761 | 0.18090 |
| C | -1.63170 | -1.57700 | -0.37164 |
| H | 0.14300 | -2.81765 | -0.31551 |
| H | -0.32094 | -2.15566 | 1.26334 |
| C | -2.09364 | -0.22842 | 0.15844 |
| H | -1.57900 | -1.54369 | -1.46312 |
| H | -2.36090 | -2.33764 | -0.09064 |
| N | -1.06089 | 0.79946 | -0.03721 |
| H | -2.98518 | 0.10116 | -0.37503 |
| H | -2.33462 | -0.29014 | 1.22500 |
| C | -1.43414 | 2.20451 | 0.06629 |
| H | 2.27872 | -1.11029 | 1.23155 |
| H | 2.53806 | -1.63211 | -0.45344 |
| C | 2.50074 | 0.54787 | -0.18337 |
| H | 3.29455 | 0.92588 | 0.45735 |
| H | 2.80868 | 0.61909 | -1.22981 |
| H | -2.51126 | 2.28076 | -0.06887 |
| H | -1.16819 | 2.61497 | 1.04470 |
| H | -0.95275 | 2.79057 | -0.71918 |
| H | 1.17011 | 2.25569 | -0.24887 |