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Supporting Information

NMR Study of CO_2 Capture by Butylamine and Oligopeptide KDDE in Aqueous Solution: Capture Efficiency and Gibbs Free Energy of the Capture Reaction as a Function of pH**

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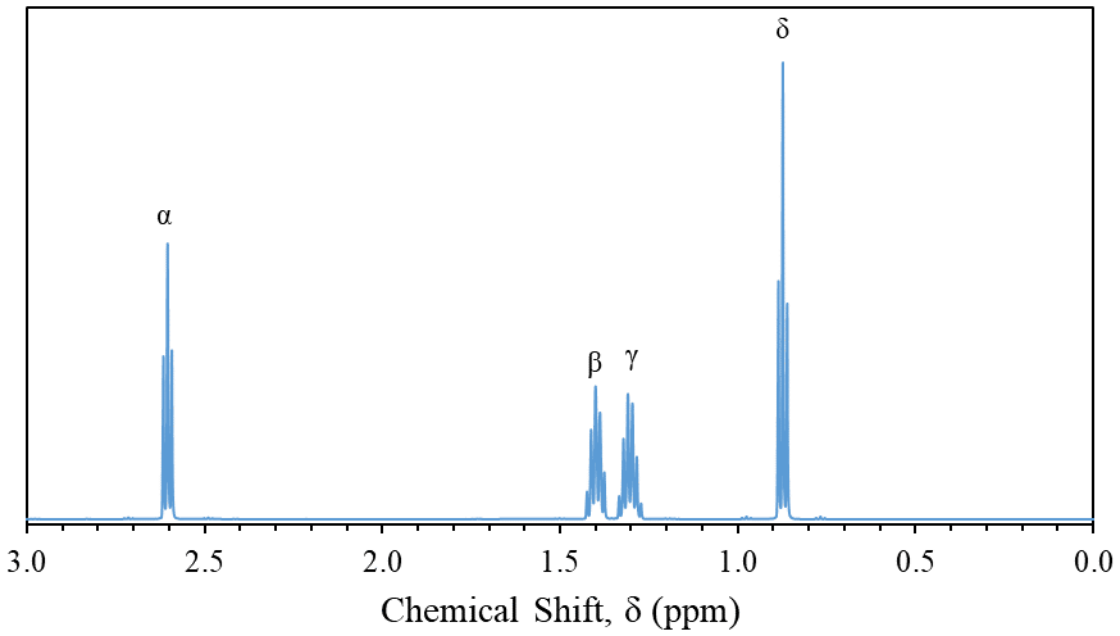

Figure S1. Measured ^{1}H NMR spectrum of butylamine in 90% H2O : 10% D2O solution with shifts at 2.61 ppm (α), 1.40 ppm (β), 1.30 ppm (γ), and 0.88 ppm (δ).

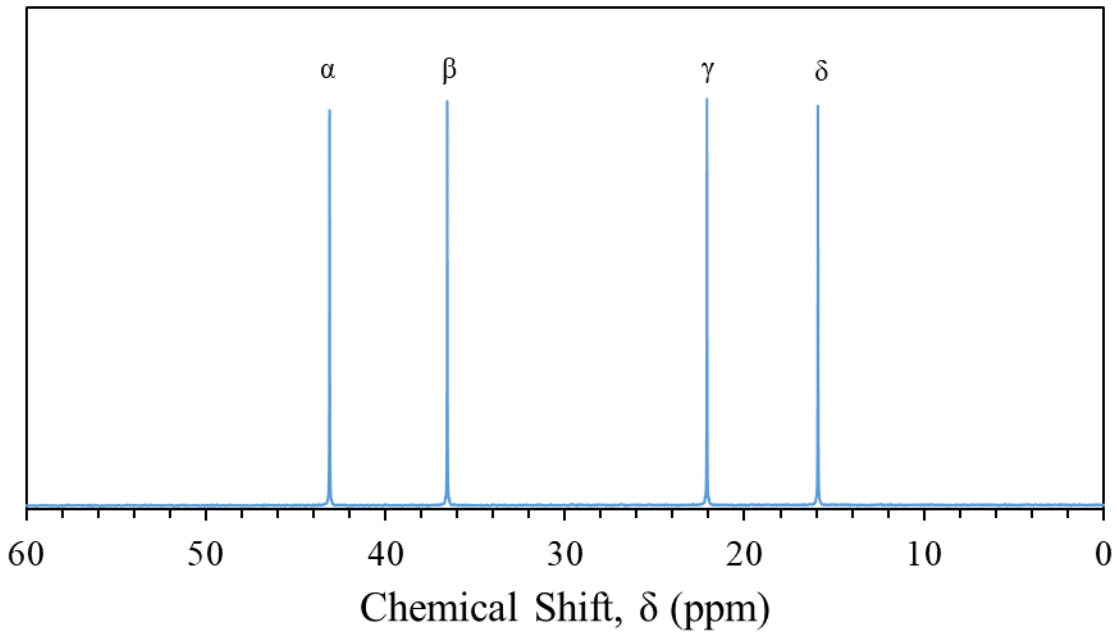

Figure S2. Measured ^{13}C NMR spectrum of butylamine in 90% H2O : 10% D2O solution with peaks at 43.09 ppm (α), 36.43 ppm (β), 22.08 ppm (γ), and 15.89 ppm (δ).

Table S1. Fraction $[CO_2]/[HCO_3^-]$ as a Function of pH.

pH	pK_2 = 6.352 (ref. [59], [60])	pK_2 = 6.18 (ref.[61])
7.0	2.25E-01	1.51E-01
8.0	2.25E-02	1.51E-02
9.0	2.25E-03	1.51E-03
9.5	7.11E-04	4.79E-04
9.8	3.56E-04	2.40E-04
10.0	2.25E-04	1.51E-04
10.1	1.79E-04	1.20E-04
10.3	1.13E-04	7.59E-05
10.5	7.11E-05	4.79E-05
10.8	3.56E-05	2.40E-05
11.2	1.42E-05	9.55E-06

Sample Preparation for Qualitative pH Profile

The NMR spectra shown in Figure S1 were collected using the noesy1dgppr pulse program provided by default with the Bruker software. This pulse program uses presaturation using the relaxation delay and the mixing time to attenuate the water signal. The values for the relaxation time and the mixing time were set to 2.00 sec and 0.01 sec, respectively. The transmitter frequency offset was assigned the value 4.703 ppm, as determined by the shift of the water signal in a preliminary measurement without presaturation. Although 1D-NOESY experiments are not strictly quantitative, the short mixing time prevents any buildup of the NOE signal and the results allow for an approximate determination of the species concentrations. However, since these measurements were taken just after the addition of acid, without sufficient time for equilibrium to be reached these data are not applicable to the Δ*G* calculations.[62-65]

In Figure S6, the region 0 – 60 ppm (top) shows the daughter α, β, γ, δ peaks and the region 150 - 180 ppm (bottom) shows the carbamate peak at 167.6 ppm. The bicarbonate peak shifts with pH between 163 and 169 ppm, and this is consistent with previous reported HCO_3^- shifts.[61] No signals were detected between 60 and 150 ppm. This agrees well with previous determinations of the ^{13}C chemical shift of some common carbamates has been determined to be 164.65 ppm for aqueous 2,2'-iminodiethanol, [66] 164.6 ppm for aqueous monoethanolamine, [67] and 166.03 ppm for ammonium carbamate in D_2O. [68] Svendsen et al. have compiled a list of several carbamates and they report the chemical shifts of the carbonyl carbons to be between 163 and 166 ppm. [69]

^{13}C Results

Table S3 list the ^1H and ^{13}C chemical shifts for the twelve samples of the qualitative data set. Again, at acidic pH, the signals from the daughter peak are diminished and not observed at pH 7.72 and below. The chemical shifts of the ^1H signals occur at the same places as the quantitative data set, and shift in the same way with pH. The chemical shifts of the ^{13}C signals for both the parent and the daughter species are mostly static over the entire pH range. Figure S7 shows the dependence of each ^{13}C shift on pH and the most notable change is the parent beta shifting slightly downfield at very high pH. The carbamate signal is present at 167.6 ppm.

Discussion of Precedents

Revision of NMR Assignments by George et al.

George et al. [70] previously studied CO_2 capture by 1-propylamine and 1-decylamine with NMR techniques in chloroform-*d* solution. They argued that capture of CO_2 is followed by ion pair formation between ammonium ion of the substrate amine and the alkylcarbamate product. Thus, for each NMR experiment, they report what they considered to be the shifts for both the carbamate portion and the ammonium portion of the ion pair. They compare these shifts to a reference spectrum of decylamine in $CDCl_3$ with peaks at 0.85 (t), 1.20 (s), 1.40 (t), 1.25 (s, broad), 2.75 (t), and 7.22 (s) ppm.

George et al. report that at low concentrations of amine only the *carbamate* portion of the aggregate appears with peaks at 2.68 (t) and 1.45 (t) ppm while at larger amine concentrations the peaks for the *ammonium* portion appear at 3.02 (t) and 1.56 (m) ppm. Thus, the authors reported that the *carbamate* portion of the NMR would appear more like the standard amine spectrum than the *ammonium*. (This claim was made even though no carbamate peak was present in the ^{13}C-NMR at those concentrations.) Surely, the peaks at 2.68 (t) and 1.45 (t) ppm must be assigned to the *ammonium* portion and the peaks at 3.02 (t) and 1.56 (m) ppm correspond to the *carbamate* portion. Therefore, with our reassignment of the results by George et al., their results for propylcarbamate formation agree well with our observation of the alpha and beta peaks of butylcarbamate at 2.99 (t) and 1.40 (m) ppm, respectively.

Our revision of their assignments also is supported by the authors' own observation that the peaks supposedly belonging to the *ammonium* decrease in intensity upon heating. Of course, this observation is much better explained by the correct assignments of these peaks to the *carbamate* in that heating simply favors the release of CO_2.

The authors also report a peak at 124 ppm in the ^{13}C NMR spectrum and tentatively attributed it to the formation of isocyanate. Rather, this peak is due to CO_2 dissolved in $CDCl_3$ solution, which has been determined to be 125.1 ppm in C_6D_6, [71] and between 125 and 129 ppm[72] in acid media.

Comparison of Lysine Sidechain Carbamylation Results Obtained by Morrow et al.

Morrow et al. measured ^{13}C- and ^1H-NMR spectra of various amino acids and their CO_2 adducts in aqueous solution. [73] The study primarily focused on glycine, but the chemical shifts were also reported for other amino acids, including lysine. The chemical shifts were reported with CS_2 as a reference for the ^{13}C-NMR spectra and 1,4-dioxane as a reference for the ^1H-

NMR spectra and positive values are associated with shifts upfield. The authors report the shift of 1,4-dioxane relative to CS_2 as 126.20 ppm. To convert the reported chemical shifts relative to TMS and follow the modern convention of positive δ values being downfield of TMS, we used $\Delta\delta$ = 192.63 ppm for ^{13}C-signal of TMS relative to CS_2 and $\Delta\delta$ = 3.75 ppm for the ^{1}H-signal of TMS relative to 1,4-dioxane.

The authors note that lysine was observed to form a carbamate at both the amine in the backbone and the amine in the side chain at pH > 9 and the ^{13}C chemical shifts for the carbamino group were 163.54 ppm and 164.4 ppm, respectively. The optimal pH reported for the carbamino adduct at the lysine ε site is 10.10. For the adduct with CO_2 bound to the amine in the backbone, the reported chemical shifts are 56.68 ppm for the α carbon and 181.13 ppm for the carbonyl carbon. For the adduct with CO_2 bound to the side chain amine group, the shifts reported are 40.92 ppm for the Cα and 181.44 ppm for the carboxyl carbon. Their assignment of the signal at 164.4 ppm to the sidechain carbamate-C agrees well with our assignments of the carbamate-C signals at 167.62 ppm ($BuNH_2$) and 167.49 ppm (KDDE). Their assignment of the signal at 40.92 ppm to Cα also agrees well with our assignments of the Cα signals at 43.87 ppm ($BuNH_2$) and 43.79 ppm (KDDE).

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Table S2. pH Profile (NOESY) of Butylamine in 90% H_2O : 10% D_2O Solution with HCO_3^- – ^1H NMR Spectra

Assignment	pH											
	10.47		10.30		10.04		9.79		9.50		9.24	
	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max
Parent												
α	2.89	2.91	2.92	2.94	2.94	2.96	2.96	2.98	2.97	2.99	2.97	3.00
β	1.55	1.60	1.57	1.62	1.58	1.63	1.59	1.65	1.60	1.65	1.60	1.65
γ	1.33	1.41	1.34	1.39	1.34	1.41	1.35	1.43	1.35	1.43	1.36	1.41
δ	0.90	0.92	0.90	0.92	0.90	0.92	0.91	0.94	0.91	0.94	0.91	0.94
Daughter												
α	2.97	3.00	2.97	3.00	2.97	3.00	2.98	3.01	2.99	3.01	a	3.01
β	1.38	1.43	1.39	1.43	1.39	1.43	1.43	1.44	1.42	1.44	1.39	1.44
γ	1.28	1.33	1.27	1.33	1.27	1.33	1.28	1.34	1.28	1.34	1.28	1.34
δ	0.87	0.89	0.87	0.89	0.87	0.89	0.87	0.90	0.87	0.90	0.87	0.90

Assignment	pH											
	8.90		8.71		8.39		7.72		6.98		6.73	
	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max
Parent												
α	2.97	3.00	2.97	3.00	2.98	3.00	2.98	3.00	2.98	3.00	2.98	3.00
β	1.60	1.65	1.60	1.65	1.60	1.65	1.60	1.65	1.60	1.65	1.60	1.65
γ	1.35	1.41	1.35	1.41	1.35	1.40	1.35	1.41	1.35	1.41	1.35	1.41
δ	0.90	0.93	0.90	0.93	0.90	0.93	0.90	0.93	0.90	0.93	0.90	0.93
Daughter												
α	u.p.[a]		u.p.		u.p.		NO[a]		NO		NO	
β	1.39	1.43	1.41	1.43	u.p.	1.42	NO		NO		NO	
γ	1.27	1.33	1.27	1.33	1.28	1.32	NO		NO		NO	
δ	0.87	0.89	0.87	0.89	0.87	0.89	NO		NO		NO	

[a] u.p.= under parent peak, NO = not observed.

Assignment	pH											
	10.47		10.30		10.04		9.79		9.50		9.24	
	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max
Parent												
α	2.89	2.91	2.92	2.94	2.94	2.96	2.96	2.98	2.97	2.99	2.97	3.00
β	1.55	1.60	1.57	1.62	1.58	1.63	1.59	1.65	1.60	1.65	1.60	1.65
γ	1.33	1.41	1.34	1.39	1.34	1.41	1.35	1.43	1.35	1.43	1.36	1.41
δ	0.90	0.92	0.90	0.92	0.90	0.92	0.91	0.94	0.91	0.94	0.91	0.94
Daughter												
α	2.97	3.00	2.97	3.00	2.97	3.00	2.98	3.01	2.99	3.01	a	3.01
β	1.38	1.43	1.39	1.43	1.39	1.43	1.43	1.44	1.42	1.44	1.39	1.44
γ	1.28	1.33	1.27	1.33	1.27	1.33	1.28	1.34	1.28	1.34	1.28	1.34
δ	0.87	0.89	0.87	0.89	0.87	0.89	0.87	0.90	0.87	0.90	0.87	0.90

Assignment	pH											
	8.90		8.71		8.39		7.72		6.98		6.73	
	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max
Parent												
α	2.97	3.00	2.97	3.00	2.98	3.00	2.98	3.00	2.98	3.00	2.98	3.00
β	1.60	1.65	1.60	1.65	1.60	1.65	1.60	1.65	1.60	1.65	1.60	1.65
γ	1.35	1.41	1.35	1.41	1.35	1.40	1.35	1.41	1.35	1.41	1.35	1.41
δ	0.90	0.93	0.90	0.93	0.90	0.93	0.90	0.93	0.90	0.93	0.90	0.93
Daughter												
α	u.p.[a]		u.p.		u.p.		NO[a]		NO		NO	
β	1.39	1.43	1.41	1.43	u.p.	1.42	NO		NO		NO	
γ	1.27	1.33	1.27	1.33	1.28	1.32	NO		NO		NO	
δ	0.87	0.89	0.87	0.89	0.87	0.89	NO		NO		NO	

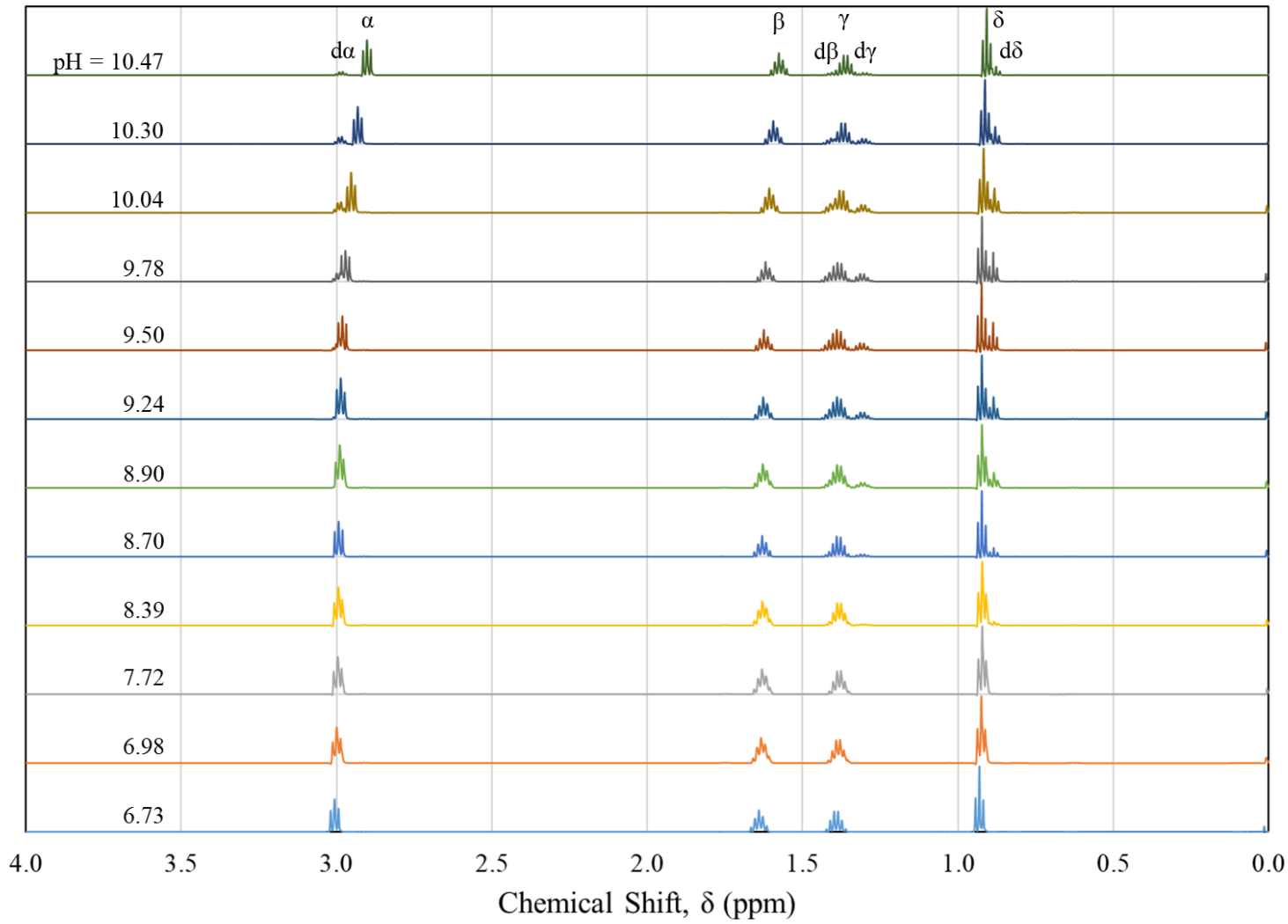


Figure S3. ^{1}H NMR pH profile using the NOESY water suppression technique "noesygppr1d" for butylamine in 90% H_2O : 10% D_2O solution with added HCO_3^-.

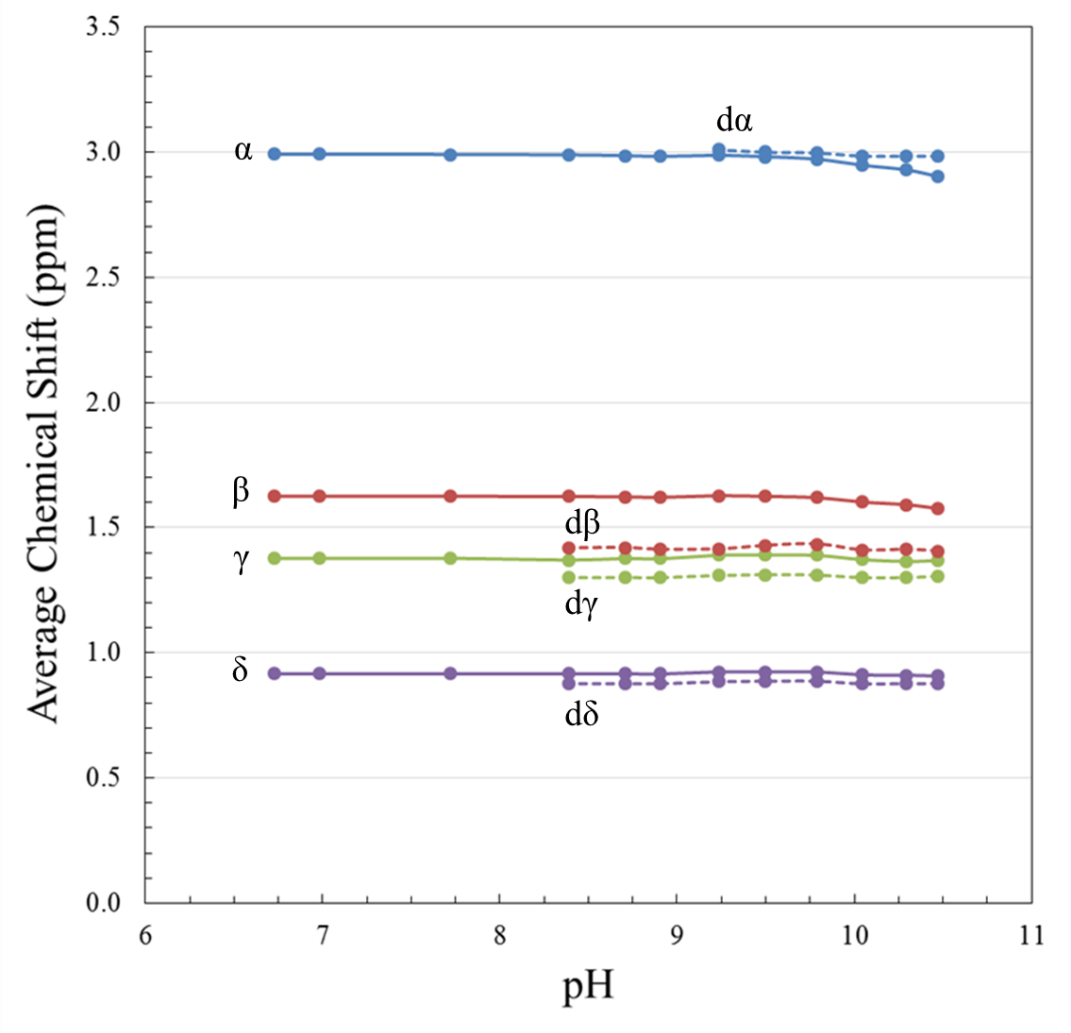


Figure S4. Chemical shift as a function of pH for the ^{1}H NMR of butylamine in 90% H_2O : 10% D_2O with HCO_3^-. The color of the line corresponds to the assignment: Blue = α, Red = β, Green = γ, Purple = δ. Solid lines show the parent species and dashed lines show the daughter species.

Table S3. pH Profile of Butylamine – ^{13}C NMR Spectra

	pH											
Assign.	10.47	10.30	10.04	9.79	9.50	9.24	8.90	8.71	8.39	7.72	6.98	6.73
Parent												
α	42.33	42.27	42.24	42.22	42.21	42.14	42.14	42.14	42.14	42.14	42.14	42.14
β	32.67	32.32	32.08	31.90	31.78	31.65	31.60	31.56	31.53	31.51	31.51	31.51
γ	21.77	21.74	21.73	21.71	21.70	21.63	21.63	21.62	21.62	21.62	21.62	21.62
δ	15.57	15.54	15.53	15.51	15.50	15.43	15.43	15.42	15.42	15.42	15.42	15.42
Daughter												
α	43.86	43.86	43.86	43.86	43.86	43.80	43.80	43.80	43.80	NO	NO	NO
β	34.50	34.50	34.50	34.50	34.50	34.44	34.44	34.44	34.44	NO	NO	NO
γ	22.12	22.12	22.12	22.12	22.12	22.06	22.06	22.06	22.06	NO	NO	NO
δ	15.89	15.89	15.90	15.90	15.90	15.84	15.84	15.84	15.84	NO	NO	NO
Carbamate	167.60	167.60	167.60	167.60	167.60	167.54	167.54	167.54	NO[a]	NO	NO	NO
HCO_3^-	168.98	168.21	167.35	166.33	165.45	164.68	164.11	163.69	163.29	162.96	162.90	162.90

a) NO = Not observed.

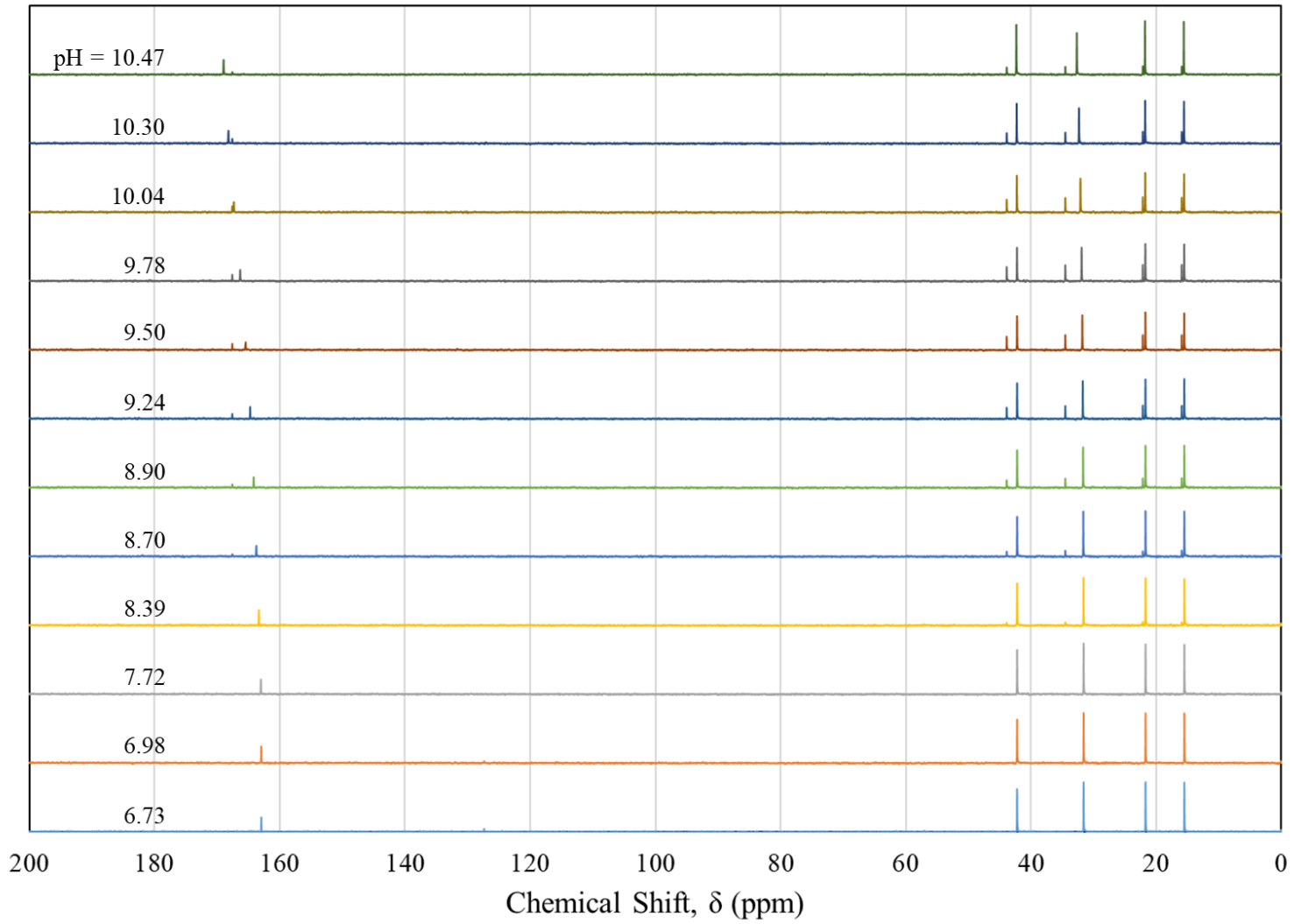
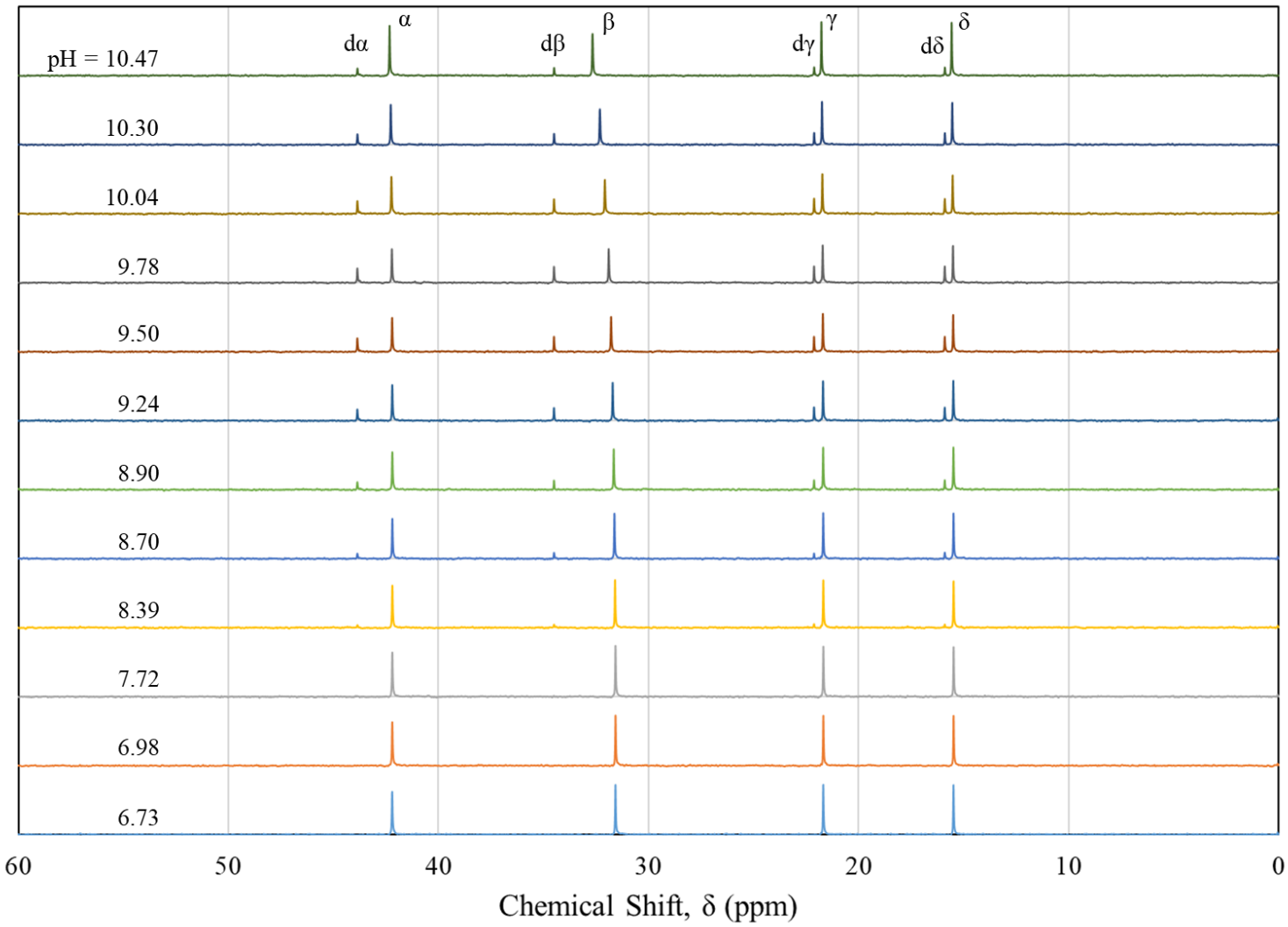


Figure S5. Full ^{13}C NMR spectra for butylamine in 90% H_2O : 10% D_2O solution with added HCO_3^-.


pH = 10.47
10.30
10.04
9.78
9.50
9.24
8.90
8.70
8.39
7.72
6.98
6.73
dα
α
dβ
β
dγ
γ
dδ
δ
60
50
40
30
20
10
0
Chemical Shift, δ (ppm)

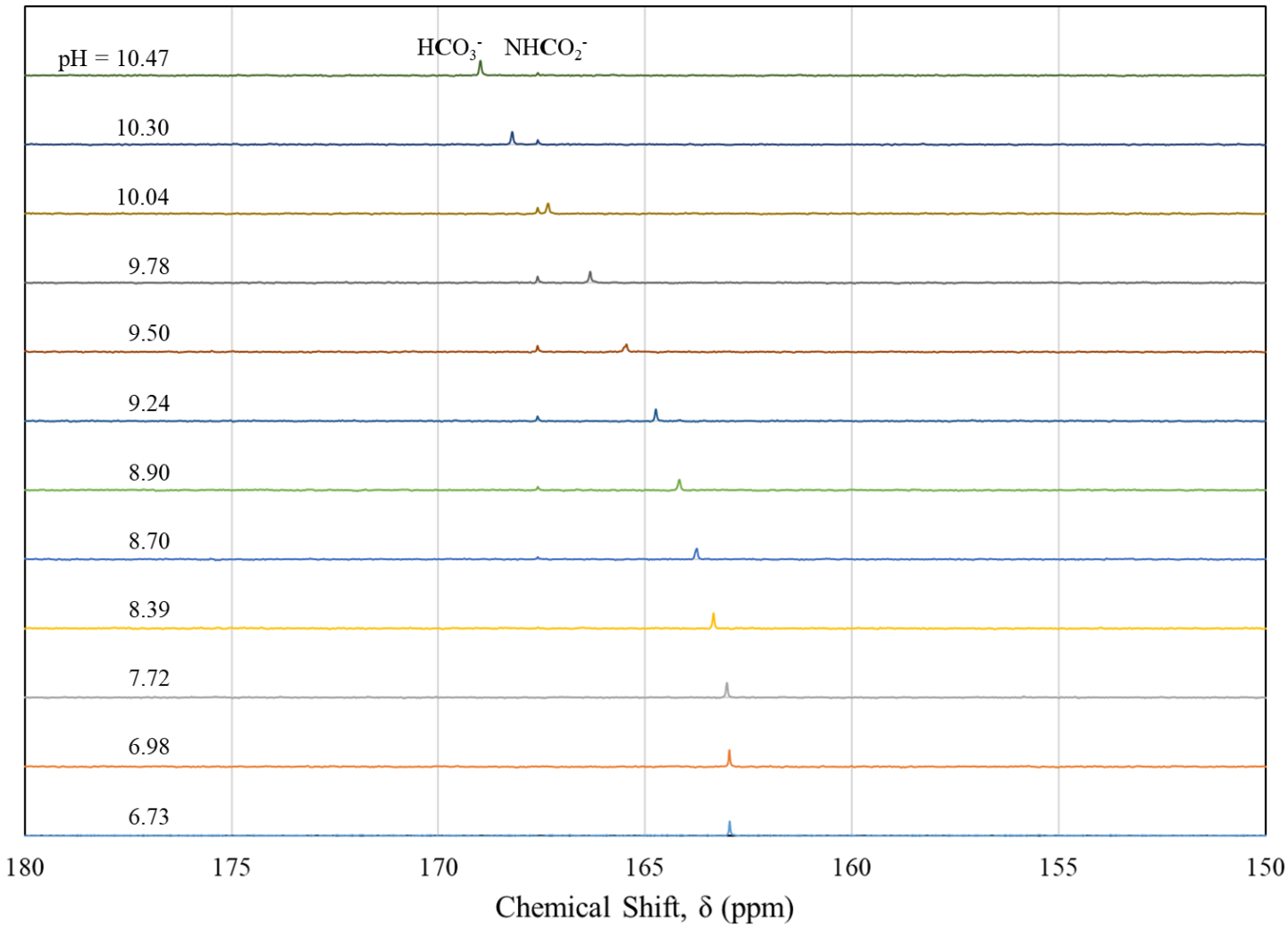


Figure S6. ^{13}C NMR of butylamine in 90% H_2O : 10% D_2O solution with added HCO_3^- at the pH values studied. Top: 0 – 60 ppm. Bottom: 150 to 180 ppm.

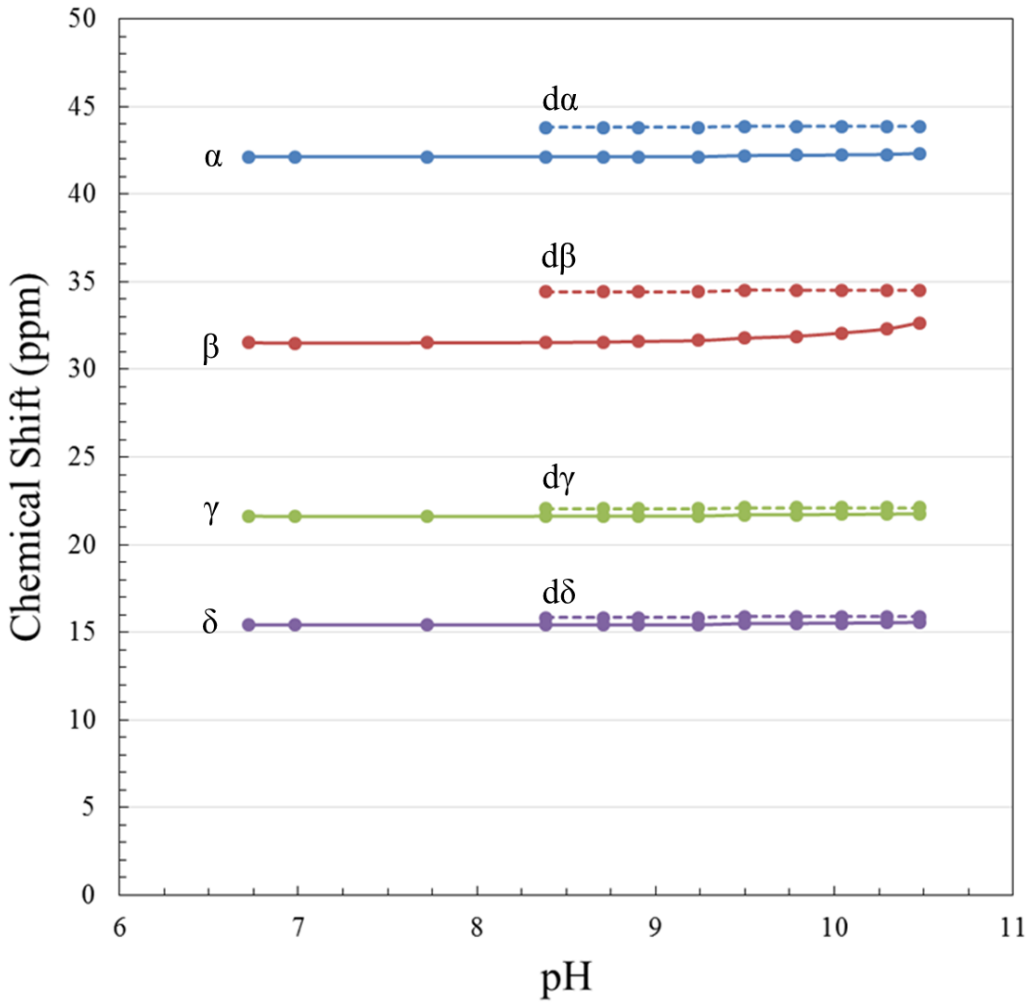


Figure S7. Chemical Shift as a function of pH for the ^{13}C NMR of butylamine in 90% H_2O : 10% D_2O with HCO_3^-. The color of the line corresponds to the assignment: Blue = α, Red = β, Green = γ, Purple = δ. Solid lines show the parent species and dashed lines show the daughter species. The carbamate peak at 167.6 is also rather static across the full pH range, but is not shown here for reasons of scale.

Evaluation of Equation 16

To evaluate Eq. 16, we determined the energies of the parent carbamic acid and its carbamate, H_2NCOOH and H_2NCOO^-, and of their alkyl substituted analogs, R−HNCOOH and R−HNCOO$^-$. All structures were optimized using the Gaussian16 software[74] with the APFD[75] method of density functional theory. Justification of computational level can be found in the previous published computational study of the CO_2 capture by amine.[76] The calculations were performed with the 6-311G* basis set[77,78] and the diffuse function augmented 6-311+G* basis set.[79] The isodesmic reaction R6 was evaluated for the gas phase and with the solvation model SMD.[80] The SMD(APFD) calculations were applied to reaction R6 as well as to the analogous reactions in which every molecule was complexed by two explicit water molecules. Total energies and thermodynamic properties are collected in Table S5 in Supporting Information 1 along with Cartesian Coordinates of all optimized structures. The most relevant results are shown in Table S6 and include the reaction energies ΔG_{R6} and the pK_5(R) values derived by Eq. 16. Figure S8 shows molecular models of alkylcarbamic acid and alkylcarbamate.

Initial calculations were performed for R = Me and these results are provided at the top of Table S6. The gas phase energies computed with the 6-311G* basis set favors the formation of the alkylated anion by about 1.32 kcal/mol. However, by adding diffuse functions to the heavy atoms, the favorability is reversed, and the equilibrium lays on the side of the non-alkylated anion with a preference of 0.62 kcal/mol. Estimating bulk solvation with the SMD solvation model, we observe the same basis set effect along with a shift in equilibrium in favor of the parent carbamate; with ΔG_{R6} values of zero and 1.5 kcal/mol at the levels SMD(AFPD/6-311G*) and SMD(AFPD/6-311+G*), respectively.

Because the solvation effects are significant, we sought to improve the accuracy of the reaction energies by adding two explicit water molecules to each carbamic acid and carbamate. We performed these calculations with the 6-311G* basis set as well with the 6-311+G* basis set on all molecules of reaction R6. While the addition of diffuse functions to anions is warranted and necessary, the presence of diffuse functions on the explicit solvent molecules is not necessary and could give rise to basis set superposition error (BSSE).[81] Hence, the structures were re-optimized using a new theoretical level that employs the 6-311+G* basis set on the carbamic acid and carbamate structures and the 6-311G* basis set on the explicit solvent water molecules. We denote the choice of this partial diffuse function augmented basis set as PDFA for brevity in the resulting theoretical level as SMD(APFD/PDFA), and this level was employed to study reaction R6 for the alkyl systems with R = Me, Et, Pr and Bu (Table S6, bottom). For the butyl systems, the calculated reaction energy is 0.21 kcal/mol in favor of the formation of butylcarbamic acid/non-alkylated carbamate; this is our best estimate of the reaction energy ΔG_{R6}(Bu) and gives pK_a(Bu) = 5.89 for reaction R5a. The accuracy of pK_a(Bu) value needs to be taken with all necessary caution because of the significant variations with the length of the alkyl chain and uncertainties associated with the theoretical model. Perhaps the most important results of our analysis are (a) that the presence of a long alky chain increases the pK_a compared to the parent system and (b) that the increase is very modest. The pK_a(R) values of carboxylic acids are 4.76 (Me), 4.87 (Et), 4.83 (Pr), 4.83 (Bu), and 4.85 (Pe),[82] and based on their convergence it would be well justified to use pK_a(Bu) = 5.89 in the analyses of both the butylamine and the KDDE system.

Carbamic Acid: Neutral or Zwitterion?

The overall carbamylation reaction involves the addition of CO_2 to an alkylamine and the formation of the alkylcarbamate, and it is the combination of reactions R1 and R5. We could also have formulated the overall reaction as the combination of reactions R1-zw and R5-zw, and in fact, the latter is the more likely reaction path for carbamate formation. The respective equilibrium constants K_n and $K_{n\text{-}zw}$ are related by the tautomerization reaction R7.

R–NH–COOH ⇄ R–NH_2^+–COO^-	(R7)
K_7(R) = [R–NH_2^+–COO^-]/[R–NH–COOH]	(Eq. 17)
R–NH_2 + CO_2 ⇄ R–NH_2^+–COO^-	(R1-zw)
$K_{1\text{-}zw}$(R) = [R–NH_2^+–COO^-]/([R–NH_2][CO_2])	(Eq. 1-zw)
$\Delta G_{1\text{-}zw}$(R) = ΔG_1(R) + ΔG_7(R)	(Eq. 18)
R–NH_2^+–COO^- ⇄ R–NH–COO^- + H^+	(R5-zw)
$K_{5\text{-}zw}$(R) = [H^+][R–NH–COO^-]/[R–NH_2^+–COO^-]	(Eq. 5-zw)
$\Delta G_{5\text{-}zw}$(R) = ΔG_5(R) - ΔG_7(R)	(Eq. 19)

We attempted to estimate the reaction energy for reaction R7 at the same levels that we employed for the evaluation of the isodesmic reactions R6. The energy data are included in Table S5 in Supporting Information 1 along with the Cartesian Coordinates of stationary structures. Molecular models of the zwitterions are included in Figure S8.

Our calculations estimate preferences for the carbamic acid form over the zwitterion form with ΔG_7(R) values of 4.44 (methyl), 2.78 (ethyl), 3.22 (propyl) and 2.98 (butyl) kcal/mol. The quality of the ΔG_7(R) values is not comparable to the accuracy of ΔG_6(R) values for several reasons. First of all, reaction R7 is not an isodesmic reaction. While the specific solvation pattern is essentially retained between the carbamic acid and carbamate, the specific solvation modes certainly differ for the tautomers. Moreover, the zwitterion might require more than two water molecules in its first solvent shell. Therefore, we determined ΔG_1(R) based on an accurate estimate of ΔG_5(R), and $\Delta G_{1\text{-zw}}$(R) and $\Delta G_{5\text{-zw}}$(R) can be derived once more accurate computational and/or experimental values for ΔG_7(R) will become available.

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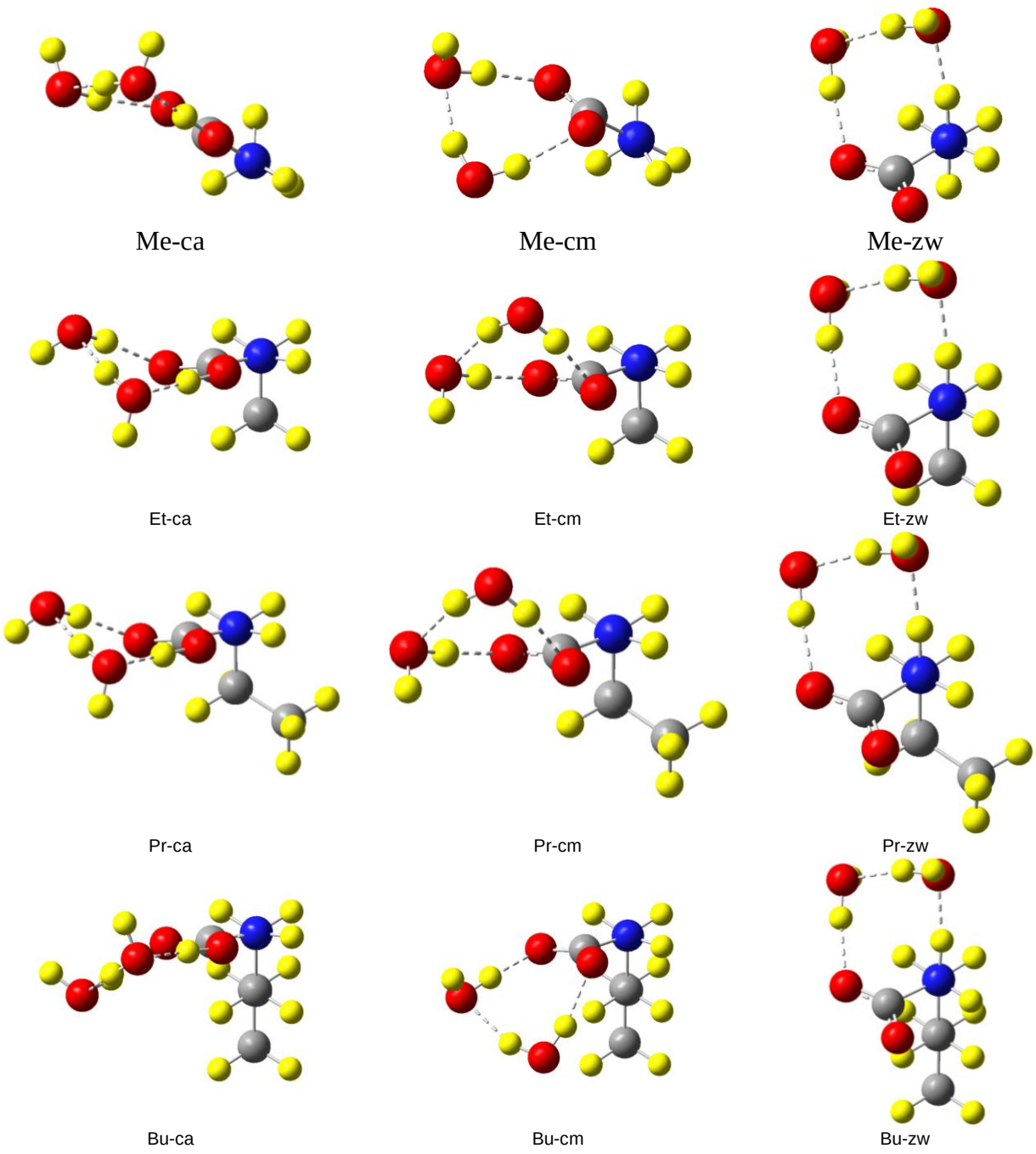

Figure S8. Molecular models of alkylcarbamic acid, alkylcarbamate, and of the zwitterion of alkylcarbamic acid computed with two explicit water molecules at the SMD(APFD) level with partial diffuse function (SMD(APFD/6-311G*) applied on the two explicit water molecules and SMD(APFD/6-311+G*) applied on the rest of atoms).

Table S4. Energies and Thermodynamic Properties[a] **for Carbamates and Carbamic Acids**

Species	Energy	*VZPE*	*TE*	*S*	*v*	*μ*	U_{298}	G_{298}
Gas Phase, APFD/6-311G*								
H_2NCOO^-	-244.432099	24.60	26.92	64.24	412.64	3.48	-244.389201	-244.418777
H_2NCOOH	-245.009527	32.58	35.34	67.14	152.44	2.39	-244.953206	-244.984163
Me−NHCOOH	-284.292018	50.62	54.19	75.40	61.74	2.34	-284.205656	-284.240535
Me−$NHCOO^-$	-283.715725	41.88	45.12	72.36	150.99	4.89	-283.643820	-283.677255
Gas Phase, APFD/6-311+G*								
H_2NCOO^-	-244.459244	24.53	26.86	64.25	418.35	3.98	-244.416448	-244.446030
H_2NCOOH	-245.018704	32.36	35.18	67.86	107.57	2.50	-244.962638	-244.993935
Me−NHCOOH	-284.300690	50.45	54.06	76.47	38.27	2.48	-284.214534	-284.249919
Me−$NHCOO^-$	-283.739251	41.83	45.12	72.86	124.51	5.66	-283.667353	-283.701027
Solvation, SMD(APFD/6-311G*)								
H_2NCOO^-	-244.556676	24.45	26.78	64.29	460.00	5.85	-244.513999	-244.543601
H_2NCOOH	-245.026817	32.02	34.87	68.45	80.08	3.39	-244.971248	-245.002824
Me−NHCOOH	-284.307332	50.08	53.73	75.54	75.82	3.54	-284.221706	-284.256654
Me−$NHCOO^-$	-283.836241	42.12	45.41	72.63	135.01	8.01	-283.763884	-283.797448
Solvation, SMD(APFD/6-311+G*)								
H_2NCOO^-	-244.580690	24.16	26.54	64.48	468.35	6.60	-244.538396	-244.568087
H_2NCOOH	-245.037169	31.96	34.71	66.97	177.07	3.66	-244.981849	-245.012723
Me−NHCOOH	-284.317323	49.85	53.55	76.22	57.75	3.83	-284.231994	-284.267265
Me−$NHCOO^-$	-283.858792	41.95	45.25	72.62	142.18	9.07	-283.786675	-283.820235

a) *E* and zero-point vibrational energy in Hartree, *TE* in kcal/mol, *S* in cal mol^{-1} K^{-1}, *μ* in Debye, and *H* and *G* in Hartree.

Table S5. Energies and Thermodynamic Properties[a] for Carbamates, Carbamic Acids and Carbamic Acid Zwitterions with Explicit Solvation

Species	Energy	*VZPE*	*TE*	*S*	*v*	*μ*	U_{298}	G_{298}
Solvation, SMD(APFD/6-311G*), Explicit Water								
H_2NCOO^-	-397.367416	55.69	61.38	93.79	34.95	6.97	-397.269609	-397.313227
H_2NCOOH	-397.836607	63.79	69.65	93.92	37.72	3.16	-397.725611	-397.769290
Me−NHCOOH	-437.117189	81.85	88.58	101.86	38.58	3.59	-436.976028	-437.023478
Me−$NHCOO^-$	-436.647286	73.51	80.15	102.55	25.62	8.96	-436.519565	-436.567343
Solvation, SMD(APFD/6-311+G*), Explicit water								
H_2NCOO^-	-397.396721	55.11	60.90	94.97	34.13	7.48	-397.299671	-397.343848
H_2NCOOH	-397.854283	63.32	69.26	94.42	36.57	2.18	-397.743910	-397.787827
Me−NHCOOH	-437.134496	81.34	88.17	102.32	33.89	2.55	-436.993991	-437.041660
Me−$NHCOO^-$	-436.675589	73.12	79.80	102.53	31.60	9.29	-436.548421	-436.596192
Solvation, Partial Diffuse Function,[b] Explicit Water								
H_2NCOO^-	-397.385930	55.67	61.40	93.90	33.18	4.30	-397.288078	-397.331747
H_2NCOOH	-397.846731	63.65	69.46	93.44	36.97	2.82	-397.736040	-397.779491
Me−NHCOOH	-437.127290	81.52	88.29	101.97	34.01	4.25	-436.986596	-437.034102
Me−$NHCOO^-$	-436.665340	73.33	80.04	102.29	30.11	6.31	-436.537785	-436.585443
Me−NH_2^+−COO^-	-437.123239	82.88	89.44	99.48	35.44	8.45	-436.980709	-437.027027
Et−NHCOOH	-476.418993	99.83	107.19	107.04	33.10	4.39	-476.248177	-476.298091
Et−$NHCOO^-$	-475.957063	91.35	98.75	109.07	23.25	9.83	-475.799697	-475.850575
Et−NH_2^+−COO^-	-476.416929	100.93	108.18	105.39	37.35	8.55	-476.244527	-476.293656
Pr−NHCOOH	-515.708208	117.67	125.84	115.12	20.90	4.51	-515.507677	-515.561431
Pr−$NHCOO^-$	-515.246461	109.50	117.61	115.13	24.71	11.79	-515.059038	-515.112792
Pr−NH_2^+−COO^-	-515.706316	118.88	126.97	112.11	45.94	8.51	-515.503978	-515.556299
Bu−NHCOOH	-554.997037	135.45	144.54	123.00	22.85	3.62	-554.766698	-554.824195
Bu−$NHCOO^-$	-554.535645	127.20	136.25	123.22	21.22	11.45	-554.318517	-554.376116
Bu−NH_2^+−COO^-	-554.995550	136.73	145.70	120.03	42.49	8.60	-554.763359	-554.819443

a) *E* in Hartree, zero-point vibrational energy and *TE* in kcal/mol, *S* in cal mol^{-1} K^{-1}, *μ* in Debye, and *U* and *G* in Hartree.

b) Partial Diffuse Function means SMD(APFD/6-311G*) applied on the two explicit water molecule and SMD(APFD/6-311+G*) applied on the rest of atoms.

Table S6. **Thermochemistry for the Isodesmic Reaction R6 Calculated at APFD with Various Basis Sets and Solvation Models and pKa Values for the Alkylcarbamic Acid**

R Group	Model	Basis Set		ΔG_{R6}	$T \cdot \Delta S_{R6}$	pK_a
		carbamic acid and carbamate	explicit water			
Methyl	Gas Phase	6-311G*		-1.32	-0.04	4.77
		6-311+G*		0.62	0.002	6.19
	SMD Solvation	6-311G*		-0.01	0.37	5.73
		6-311+G*		1.50	-0.33	6.84
	SMD Solv. + 2 H_2O	6-311G*	6-311G*	0.04	0.24	5.77
		6-311+G*	6-311+G*	0.93	-0.10	6.42
		6-311+G*	6-311G*	0.57	-0.04	6.16
Ethyl	SMD Solv. + 2 H_2O	6-311+G*	6-311G*	-0.14	0.47	5.64
Propyl				0.56	-0.14	6.15
Butyl				0.21	-0.07	5.89

Coordinates of small alkylamines and alkylcarbamic acids for study of R-group effects

Gas phase, APFD/6-311G*

Carbamic acid, $H_2N-COOH$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.041838	0.126221	-0.001047
2	7	0	1.269668	-0.216497	-0.026049
3	1	0	1.949838	0.514108	0.068933
4	1	0	1.555003	-1.172711	0.079411
5	8	0	-0.484998	1.249814	0.003240
6	8	0	-0.816619	-0.987979	0.001475
7	1	0	-1.728552	-0.677923	0.002564

Carbamate, H_2N-COO^-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.184473	-0.000000	-0.012005
2	7	0	1.288001	0.000015	-0.110221
3	1	0	1.653982	0.833343	0.333729
4	1	0	1.653979	-0.833316	0.333721
5	8	0	-0.701086	1.136024	0.011008
6	8	0	-0.701055	-1.136041	0.011008

Methylcarbamic acid

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.521208	0.109189	-0.000002
2	7	0	-0.623186	-0.611819	-0.000005
3	1	0	-0.542367	-1.614168	0.000002
4	8	0	1.596290	-0.722746	0.000002
5	8	0	0.615659	1.316319	-0.000000
6	6	0	-1.921493	0.012624	0.000003
7	1	0	-1.770677	1.090945	-0.000039
8	1	0	-2.495499	-0.260479	-0.890454
9	1	0	-2.495466	-0.260418	0.890500
10	1	0	2.372432	-0.152605	0.000004

Methylcarbamate

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.668807	0.066267	-0.031443
2	7	0	-0.594749	-0.647752	-0.261189
3	1	0	-0.503445	-1.591102	0.089491
4	8	0	1.650932	-0.690027	0.116012
5	8	0	0.593406	1.312441	-0.036607
6	6	0	-1.813131	0.015234	0.113068
7	1	0	-1.696571	1.062628	-0.170023
8	1	0	-2.684629	-0.404110	-0.414356
9	1	0	-2.040869	-0.001464	1.198219

Solvation: SMD(APFD/6-311G*)

Carbamic acid $H_2N-COOH$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.261493	-0.240951	-0.008153
2	6	0	-0.030720	0.115381	-0.000061
3	8	0	-0.454854	1.263759	0.000837
4	8	0	-0.844546	-0.967049	0.000520
5	1	0	1.965944	0.475604	0.022362
6	1	0	1.538682	-1.207435	0.023403
7	1	0	-1.755556	-0.647481	0.000814

Carbamate H_2N-COO^-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.264345	0.000001	-0.088740
2	6	0	-0.142527	-0.000000	-0.002936
3	8	0	-0.712402	1.127811	0.007873
4	8	0	-0.712399	-1.127812	0.007873
5	1	0	1.701577	0.841428	0.256414
6	1	0	1.701579	-0.841425	0.256414

Methylcarbamic acid

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.515205	0.095104	-0.004762
2	7	0	-0.610413	-0.630663	-0.030376
3	1	0	-0.538647	-1.633236	0.033103
4	8	0	1.620232	-0.691480	0.009334
5	8	0	0.569896	1.320099	-0.002423
6	6	0	-1.906660	0.009282	0.012741
7	1	0	-2.011560	0.727390	-0.802657
8	1	0	-2.674291	-0.754310	-0.098472
9	1	0	-2.067929	0.532618	0.959105
10	1	0	2.393025	-0.113087	0.018389

Methylcarbamate

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.823607	0.020016	0.087254
2	1	0	1.904105	0.360511	1.128623
3	1	0	1.944480	0.892311	-0.556267
4	7	0	0.573510	-0.648514	-0.205312
5	6	0	-0.635875	0.045054	-0.026386
6	8	0	-1.679292	-0.662772	0.087755
7	8	0	-0.590876	1.307916	-0.025678
8	1	0	2.652635	-0.661235	-0.113671

9	1	0	0.519153	-1.603562	0.116672

Solvation: SMD(APFD/6-311G*) and 2 explicit water molecules

Carbamic acid $H_2N-COOH$ H2NCOOH_2H2Oa_nodif_02.log

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.506200	-0.146806	-0.106964
2	1	0	-2.985286	-0.984392	0.176199
3	1	0	-3.043748	0.682823	-0.294528
4	6	0	-1.173297	-0.077808	0.045015
5	8	0	-0.685729	1.121042	-0.256442
6	8	0	-0.487638	-1.040336	0.411548
7	1	0	1.192558	-1.279040	0.030780
8	8	0	2.150740	-1.269918	-0.172397
9	1	0	2.218972	-1.424799	-1.119005
10	1	0	0.309680	1.171331	-0.103506
11	8	0	1.868616	1.358965	0.110700
12	1	0	1.977355	1.551580	1.046855
13	1	0	2.145732	0.418968	-0.005405

Carbamate H_2N-COO^- H2NCOO_2H2O_nodif.log

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.495086	0.029340	-0.147727
2	1	0	-3.010509	-0.634317	0.409212
3	1	0	-2.918974	0.941735	-0.211705
4	6	0	-1.117182	0.017090	0.028355
5	8	0	-0.488083	1.050958	-0.353339
6	8	0	-0.605371	-1.034148	0.511546
7	1	0	1.013583	-1.366178	-0.054160
8	8	0	1.939101	-1.419677	-0.371176
9	1	0	2.241558	-0.500223	-0.276779
10	1	0	1.126923	1.189919	0.000207
11	8	0	2.096749	1.270360	0.194967
12	1	0	2.176941	1.121209	1.141199

Methylcarbamic acid H3CNHCOOH_2H2Ob_01.log

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.994145	0.462691	0.203684
2	1	0	-2.305376	1.388093	0.451604
3	6	0	-0.682009	0.270654	0.005114
4	8	0	0.049746	1.342149	0.305628
5	8	0	-0.215614	-0.800898	-0.407123
6	1	0	1.024345	1.194962	0.097774
7	1	0	2.651639	1.170517	-1.164837
8	1	0	2.347729	-1.652345	1.181890
9	8	0	2.576656	1.048826	-0.213502
10	1	0	2.660968	0.078355	-0.057726
11	8	0	2.306136	-1.562944	0.225295
12	1	0	1.366269	-1.382741	0.015172
13	6	0	-2.960716	-0.564435	-0.114925
14	1	0	-2.727894	-1.491693	0.411473
15	1	0	-3.944896	-0.224883	0.203111

16	1	0	-2.992814	-0.773479	-1.187753

Methylcarbamate H3CNHCOO_2H2O_01.log

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.959878	-0.452927	-0.341809
2	1	0	2.200370	-1.425045	-0.460450
3	6	0	0.610980	-0.233231	-0.120989
4	8	0	-0.173234	-1.173459	-0.465672
5	8	0	0.265431	0.879884	0.372957
6	1	0	-1.323758	1.400673	-0.142344
7	8	0	-2.255061	1.551154	-0.406246
8	1	0	-2.663199	0.692293	-0.203890
9	1	0	-1.732935	-1.100962	0.093784
10	8	0	-2.670271	-1.047130	0.416816
11	1	0	-2.601537	-0.800995	1.343532
12	6	0	2.953325	0.382526	0.296575
13	1	0	3.945144	0.072517	-0.035293
14	1	0	2.812895	1.425174	0.009033
15	1	0	2.923127	0.327463	1.391936

Gas Phase, APFD/6-311+G*

Carbamic acid $H_2N-COOH$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.040688	0.125797	-0.000017
2	7	0	1.267638	-0.221928	-0.000165
3	1	0	1.959251	0.504831	0.000468
4	1	0	1.553872	-1.184252	0.000478
5	8	0	-0.478548	1.253414	0.000022
6	8	0	-0.822164	-0.983801	0.000016
7	1	0	-1.736769	-0.678766	0.000006

Carbamate H_2N-COO^-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.178383	0.000162	-0.009706
2	7	0	1.281737	-0.001181	-0.102849
3	1	0	1.673846	0.836157	0.307191
4	1	0	1.672127	-0.839380	0.307059
5	8	0	-0.701773	1.136024	0.010242
6	8	0	-0.704207	-1.134710	0.010249

Methylcarbamic acid H3CNHCOOHb_gas_dif.log

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.521464	0.109327	-0.000003
2	7	0	-0.623402	-0.608852	-0.000001
3	1	0	-0.541320	-1.612138	0.000017
4	8	0	1.596424	-0.724132	0.000001

5	8	0	0.618646	1.317728	0.000003
6	6	0	-1.924853	0.011880	-0.000001
7	1	0	-1.783113	1.091593	0.000059
8	1	0	-2.495885	-0.265445	-0.890710
9	1	0	-2.495933	-0.265534	0.890650
10	1	0	2.379844	-0.162525	-0.000011

Methylcarbamate Me_NH_COOdgas.log

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.818557	0.014499	0.108548
2	1	0	1.993630	0.095565	1.198328
3	1	0	1.780712	1.032068	-0.282732
4	7	0	0.589896	-0.643661	-0.248919
5	6	0	-0.665513	0.064266	-0.030119
6	8	0	-1.657568	-0.687228	0.110935
7	8	0	-0.593506	1.312491	-0.034950
8	1	0	2.681080	-0.502499	-0.335581
9	1	0	0.505633	-1.594199	0.083959

Solvation: SMD(APFD/6-311+G*)

Carbamic acid $H_2N-COOH$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.260261	-0.246707	0.000009
2	6	0	-0.029046	0.112953	-0.000014
3	8	0	-0.447932	1.267264	0.000004
4	8	0	-0.850559	-0.961687	-0.000005
5	1	0	1.970348	0.466501	-0.000020
6	1	0	1.534326	-1.215833	0.000010
7	1	0	-1.764294	-0.646049	0.000046

Carbamate H_2N-COO^-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.259956	0.000000	-0.078824
2	6	0	-0.134790	-0.000000	-0.001851
3	8	0	-0.715282	1.127210	0.007006
4	8	0	-0.715282	-1.127211	0.007006
5	1	0	1.716783	0.846761	0.225390
6	1	0	1.716783	-0.846760	0.225390

Methylcarbamic acid

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.910408	0.009398	-0.000000
2	1	0	2.045038	0.631334	0.887717
3	1	0	2.045029	0.631349	-0.887708
4	7	0	0.610842	-0.627374	0.000001
5	6	0	-0.515019	0.093328	-0.000000

6	8	0	-1.620782	-0.692437	-0.000001
7	8	0	-0.573014	1.321688	-0.000000
8	1	0	2.673523	-0.766782	-0.000011
9	1	0	0.539255	-1.632985	-0.000002
10	1	0	-2.400706	-0.121667	0.000005

Methylcarbamate

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.631085	0.041637	-0.021428
2	7	0	-0.570300	-0.644345	-0.169009
3	1	0	-0.522853	-1.614334	0.105330
4	8	0	1.687881	-0.661643	0.070717
5	8	0	0.595881	1.308539	-0.019773
6	6	0	-1.833873	0.021063	0.070903
7	1	0	-1.980486	0.837848	-0.637524
8	1	0	-2.643257	-0.695961	-0.073973
9	1	0	-1.914679	0.431497	1.084830

Solvation: SMD(APFD/6-311+G*) and 2 explicit water molecules

Carbamic acid $H_2N-COOH$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.984129	-0.597437	0.062949
2	6	0	0.652763	-0.254931	-0.020331
3	8	0	-0.168124	-1.203610	-0.252030
4	8	0	0.337610	0.959758	0.162576
5	1	0	2.212225	-1.509484	-0.302007
6	1	0	-1.315266	1.450590	-0.051014
7	8	0	-2.272079	1.658187	-0.146579
8	1	0	-1.821634	-1.102094	-0.012522
9	8	0	-2.806939	-1.047226	0.085011
10	1	0	-3.003208	-1.281603	0.996930
11	1	0	-2.696998	0.783746	-0.074918
12	6	0	3.025908	0.406118	0.036511
13	1	0	2.935580	1.081723	0.888756
14	1	0	3.993506	-0.092185	0.104949
15	1	0	3.011117	1.007364	-0.879720

Carbamate H_2N-COO^- H2NCOO_2H2O_04.log

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.546739	-0.114373	-0.031773
2	1	0	3.068369	0.655508	0.358058
3	1	0	2.932592	-1.029216	0.143942
4	6	0	1.167632	-0.004406	-0.012943
5	8	0	0.500434	-1.073999	-0.173471
6	8	0	0.677267	1.157304	0.119829
7	1	0	-1.037195	1.400481	-0.028732
8	8	0	-2.016279	1.471934	-0.088212
9	1	0	-2.311529	0.543954	-0.055081
10	1	0	-1.171235	-1.210297	-0.034067
11	8	0	-2.156278	-1.296373	0.017949
12	1	0	-2.355119	-1.604310	0.907186

Methylcarbamic acid H3CNHCOOH_2H2Oa_dif_01.log

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.038507	-0.489830	-0.045887
2	1	0	-2.355541	-1.445620	-0.092439
3	6	0	-0.720442	-0.262581	0.015916
4	8	0	0.002124	-1.383188	-0.024190
5	8	0	-0.235362	0.875836	0.100889
6	1	0	1.421351	1.390568	-0.061574
7	8	0	2.381271	1.559979	-0.167632
8	1	0	2.658944	2.062783	0.604361
9	1	0	0.989188	-1.207111	0.039641
10	8	0	2.593533	-1.089580	0.136104
11	1	0	2.989551	-1.527668	-0.623816
12	1	0	2.723920	-0.122402	0.006168
13	6	0	-2.998521	0.591443	-0.003916
14	1	0	-3.997693	0.167936	-0.089669
15	1	0	-2.934433	1.144802	0.935912
16	1	0	-2.844491	1.287977	-0.830745

Methylcarbamate H3CNHCOO_2H2O_dif_01.log

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.995471	-0.557164	-0.187307
2	1	0	2.212041	-1.536980	-0.086794
3	6	0	0.657116	-0.245430	-0.092618
4	8	0	-0.164833	-1.214341	-0.206047
5	8	0	0.338976	0.970890	0.073088
6	1	0	-1.324362	1.448497	-0.072912
7	8	0	-2.285201	1.651267	-0.131593
8	1	0	-2.703073	0.774966	-0.042561
9	1	0	-1.817786	-1.106518	0.028421
10	8	0	-2.802782	-1.053811	0.130922
11	1	0	-2.993368	-1.284268	1.045028
12	6	0	3.019564	0.389279	0.198367
13	1	0	3.996434	-0.072700	0.051568
14	1	0	2.974850	1.284581	-0.424014
15	1	0	2.937604	0.697429	1.246958

Partial Diffuse (APFD/6-311+G*) and (APFD/6-311G*)

Diffuse function added to the molecule, not added to the solvation waters.

Carbamic acid $H_2N-COOH$ H2NCOOH_2H2Ob_pdif_02.log

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.515445	-0.152418	-0.086276
2	1	0	2.985686	-1.027208	0.075499
3	1	0	3.052475	0.652794	-0.363948
4	6	0	1.182214	-0.083597	0.044889
5	8	0	0.697740	1.124341	-0.222369
6	8	0	0.485011	-1.051428	0.382969
7	1	0	-0.304698	1.176906	-0.076048
8	1	0	-2.003724	1.597554	1.005731

9	1	0	-2.272829	-1.488229	-1.079057
10	8	0	-1.847219	1.375653	0.082726
11	1	0	-2.144904	0.441776	-0.027116
12	8	0	-2.184017	-1.261075	-0.148628
13	1	0	-1.225533	-1.285015	0.041955

Carbamate $H_2N{-}COO^-$ NH2_COO_2waterdp.log

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.431938	0.023526	-0.215509
2	6	0	1.094413	-0.102890	0.115892
3	8	0	0.492833	-1.147519	-0.288272
4	8	0	0.573994	0.805057	0.832535
5	1	0	2.762984	-0.531840	-0.989318
6	1	0	-0.901156	1.453071	-0.007474
7	8	0	-1.744277	1.517042	-0.490586
8	1	0	-1.180047	-1.180929	-0.013982
9	8	0	-2.159934	-1.150594	0.108387
10	1	0	-2.293027	-1.047590	1.055190
11	1	0	-2.109264	0.620302	-0.378928
12	1	0	2.829528	0.947755	-0.148788

Methylcarbamic acid H3CNHCOOH_2H2Oc_pdif_03.log

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.022659	-0.467878	-0.113968
2	1	0	2.352729	-1.398766	-0.316079
3	6	0	0.702577	-0.273768	-0.000156
4	8	0	-0.011278	-1.377727	-0.219051
5	8	0	0.204499	0.827584	0.280863
6	1	0	-0.999570	-1.223252	-0.063771
7	1	0	-2.675299	2.017159	0.453919
8	8	0	-2.555255	-1.091252	0.131840
9	1	0	-2.663067	-0.125381	-0.034733
10	8	0	-2.355480	1.535947	-0.315332
11	1	0	-1.403096	1.382619	-0.154471
12	6	0	2.966950	0.611405	0.075151
13	1	0	2.905115	1.022154	1.085545
14	1	0	3.971315	0.220881	-0.079284
15	1	0	2.794009	1.417479	-0.641267
16	1	0	-2.717802	-1.219977	1.071379

Methylcarbamic acid zwitterions

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.658578	0.945669	-0.013770
2	1	0	-0.213477	1.002707	0.578778
3	6	0	1.240308	-0.464798	0.176001
4	8	0	2.220295	-0.495989	0.918445
5	8	0	0.624756	-1.349567	-0.431830
6	1	0	-1.177377	-1.295685	-0.506064
7	1	0	-1.630117	0.573436	2.159454
8	8	0	-2.140173	-1.164067	-0.418218
9	1	0	-2.424304	-0.769578	-1.248723
10	8	0	-1.742342	0.903464	1.262898
11	6	0	0.296128	1.278757	-1.407958

12	1	0	-0.493412	0.608846	-1.737170
13	1	0	-0.061296	2.307118	-1.435532
14	1	0	1.171054	1.169291	-2.046337
15	1	0	1.332793	1.614011	0.355475
16	1	0	-2.032820	0.135690	0.717876

Methylcarbamate H3CNHCOO_2H2Ob_pdif_01.log

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.932557	-0.437323	-0.128421
2	1	0	-2.166728	-1.415471	-0.055096
3	6	0	-0.618122	-0.177497	-0.447224
4	8	0	0.074886	-1.141068	-0.908509
5	8	0	-0.194061	1.009878	-0.284843
6	1	0	2.859612	1.234212	-0.851282
7	8	0	2.206726	-1.270064	0.841854
8	1	0	2.471608	-0.347572	0.669637
9	8	0	2.444697	1.355605	0.007521
10	1	0	1.475660	1.250830	-0.149826
11	6	0	-2.717557	0.492249	0.654465
12	1	0	-2.816000	1.448127	0.137321
13	1	0	-3.717982	0.079490	0.789201
14	1	0	-2.285641	0.681654	1.643728
15	1	0	1.463462	-1.393335	0.223639

Ethylcarbamic acid et_ca_pd_water.log

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.499150	-0.634093	-0.618483
2	1	0	1.737902	-1.607506	-0.740148
3	6	0	0.241364	-0.359225	-0.235720
4	8	0	-0.559707	-1.424248	-0.286507
5	8	0	-0.142213	0.768840	0.109009
6	1	0	-1.484337	-1.206034	0.060519
7	1	0	-2.951705	2.192086	0.266645
8	8	0	-2.956774	-0.940099	0.559440
9	1	0	-3.051535	-0.014679	0.232992
10	8	0	-2.711524	1.542197	-0.400650
11	1	0	-1.756020	1.375493	-0.278664
12	6	0	2.574726	0.332470	-0.471085
13	1	0	3.365331	0.041073	-1.165596
14	1	0	2.203079	1.303743	-0.803372
15	1	0	-2.904758	-0.879164	1.518236
16	6	0	3.110360	0.416463	0.948946
17	1	0	3.913985	1.156807	1.011241
18	1	0	2.323463	0.712058	1.648859
19	1	0	3.513590	-0.546986	1.275484

Ethylcarbamic acid zwitterions

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.488974	-0.046987	-0.827268
2	1	0	-0.505680	-0.038505	-1.176316
3	6	0	0.642148	1.130040	0.149970
4	8	0	1.323830	2.054261	-0.290640
5	8	0	0.045492	0.973234	1.223008

6	1	0	-1.499361	0.067101	1.344326
7	1	0	-2.507109	0.687905	-1.695277
8	8	0	-2.355910	-0.391644	1.247836
9	1	0	-2.181953	-1.314261	1.458785
10	8	0	-2.166386	-0.171786	-1.429392
11	6	0	0.763945	-1.383486	-0.231402
12	1	0	0.033697	-1.531202	0.562906
13	1	0	0.560791	-2.115965	-1.014867
14	1	0	1.107737	0.121795	-1.620110
15	1	0	-2.390221	-0.274993	-0.475148
16	6	0	2.183737	-1.483943	0.276367
17	1	0	2.379375	-0.761295	1.074046
18	1	0	2.357217	-2.483086	0.683262
19	1	0	2.907496	-1.316765	-0.526838

Ethylcarbamate et_cm_pd_water2.log

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.343924	-0.898178	-0.238042
2	1	0	1.610208	-1.727890	0.273412
3	6	0	0.159661	-0.334929	0.202800
4	8	0	-0.600830	-1.067817	0.912962
5	8	0	-0.111443	0.851835	-0.159435
6	1	0	-2.900062	1.645740	0.916056
7	8	0	-2.991956	-1.103225	-0.449081
8	1	0	-3.089046	-0.134404	-0.400271
9	8	0	-2.673323	1.608307	-0.017632
10	1	0	-1.719114	1.353235	-0.045380
11	6	0	2.443072	-0.076954	-0.716166
12	1	0	3.139379	-0.735938	-1.242603
13	1	0	2.049538	0.617983	-1.460563
14	1	0	-2.178147	-1.254605	0.066548
15	6	0	3.168675	0.677687	0.388192
16	1	0	3.985365	1.280892	-0.022414
17	1	0	2.487696	1.349744	0.918965
18	1	0	3.598690	-0.015123	1.119077

Propylcarbamic acid

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.053322	-0.276229	-0.956710
2	1	0	1.364440	-1.197248	-1.229290
3	6	0	-0.174716	-0.194546	-0.415499
4	8	0	-0.878521	-1.317617	-0.559925
5	8	0	-0.616985	0.823806	0.136907
6	1	0	-1.790468	-1.242139	-0.127941
7	1	0	-3.471287	1.893357	0.895054
8	8	0	-3.245099	-1.207449	0.475897
9	1	0	-3.436168	-0.245965	0.370272
10	8	0	-3.277091	1.432898	0.072981
11	1	0	-2.305088	1.332361	0.047215
12	6	0	2.057921	0.749225	-0.725978
13	1	0	2.800300	0.655670	-1.522971
14	1	0	1.580000	1.723096	-0.848012
15	1	0	-3.153343	-1.359162	1.421502
16	6	0	2.730406	0.644687	0.638286
17	1	0	3.407374	1.500848	0.747126
18	1	0	1.969839	0.749505	1.421388
19	6	0	3.501134	-0.655825	0.821138
20	1	0	3.994887	-0.693319	1.796934
21	1	0	2.844034	-1.529274	0.757191

22	1	0	4.275336	-0.768483	0.053950

Propylcarbamic acid zwitterions

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.071427	0.464571	-0.862976
2	1	0	-0.963408	-0.013211	-1.159481
3	6	0	-0.418641	1.420851	0.288666
4	8	0	-0.362149	2.610480	-0.019725
5	8	0	-0.715710	0.847676	1.344748
6	1	0	-1.545730	-0.742067	1.364951
7	1	0	-3.087929	-0.428538	-1.498640
8	8	0	-2.038030	-1.575675	1.236247
9	1	0	-1.379845	-2.275775	1.290172
10	8	0	-2.316829	-0.991389	-1.378131
11	6	0	0.922521	-0.584806	-0.512212
12	1	0	0.496906	-1.165468	0.305679
13	1	0	1.004551	-1.239800	-1.382621
14	1	0	0.265519	1.024013	-1.646092
15	1	0	-2.342485	-1.301772	-0.443414
16	6	0	2.263723	0.010674	-0.137275
17	1	0	2.140865	0.688675	0.716114
18	1	0	2.639076	0.616860	-0.970651
19	6	0	3.261063	-1.085308	0.210197
20	1	0	3.419336	-1.762534	-0.635389
21	1	0	4.232131	-0.663239	0.483211
22	1	0	2.910761	-1.686341	1.055627

Propylcarbamate pr_cm_pd_water.log

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.891277	-0.836150	0.549176
2	1	0	-1.221349	-1.682148	0.107078
3	6	0	0.235102	-0.307713	-0.056650
4	8	0	0.897876	-1.079728	-0.821022
5	8	0	0.558986	0.889106	0.219334
6	1	0	3.238710	1.534497	-1.181156
7	8	0	3.410531	-1.135971	0.313056
8	1	0	3.518941	-0.173186	0.202857
9	8	0	3.110632	1.558208	-0.228412
10	1	0	2.157724	1.337795	-0.087279
11	6	0	-1.922912	0.022414	1.107295
12	1	0	-2.590706	-0.615957	1.694786
13	1	0	-1.452289	0.713194	1.810226
14	1	0	2.548224	-1.295293	-0.112523
15	6	0	-2.731258	0.793415	0.066809
16	1	0	-3.450715	1.431194	0.596141
17	1	0	-2.063290	1.469691	-0.479853
18	6	0	-3.464068	-0.116799	-0.910140
19	1	0	-4.068892	0.459378	-1.617379
20	1	0	-2.766882	-0.721379	-1.499493
21	1	0	-4.135909	-0.805559	-0.385174

Butylcarbamic acid

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	0.210477	-1.573135	0.103500
2	1	0	0.210988	-2.354817	-0.535253
3	6	0	-0.888519	-0.800410	0.118245
4	8	0	-1.886982	-1.308552	-0.604370
5	8	0	-0.972604	0.259905	0.756100
6	1	0	-2.731744	-0.758267	-0.519061
7	1	0	-3.058108	2.594980	0.976829
8	8	0	-4.092160	0.033395	-0.491764
9	1	0	-3.748073	0.935027	-0.288176
10	8	0	-2.737019	2.243279	0.140961
11	1	0	-2.026238	1.612471	0.370847
12	6	0	1.479407	-1.109020	0.636385
13	1	0	1.288013	-0.625077	1.597042
14	1	0	2.086918	-1.993372	0.843057
15	1	0	-4.563273	-0.257012	0.295219
16	6	0	2.217399	-0.161846	-0.299699
17	1	0	2.409703	-0.671923	-1.252571
18	1	0	1.570842	0.694891	-0.528350
19	6	0	3.530121	0.325873	0.299921
20	1	0	3.328516	0.827373	1.255659
21	1	0	4.164754	-0.537763	0.539002
22	6	0	4.277016	1.272123	-0.630604
23	1	0	5.217310	1.617722	-0.189058
24	1	0	4.518966	0.784786	-1.581516
25	1	0	3.675658	2.158400	-0.861061

Butylcarbamic acid zwitterions

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.600898	0.472631	-0.872144
2	1	0	-1.483233	-0.045057	-1.126708
3	6	0	-0.936828	1.400943	0.305713
4	8	0	-0.967537	2.593404	0.004563
5	8	0	-1.140750	0.805819	1.371690
6	1	0	-1.897058	-0.823309	1.409847
7	1	0	-3.609051	-0.515224	-1.362918
8	8	0	-2.368746	-1.670051	1.290574
9	1	0	-1.685085	-2.347340	1.277809
10	8	0	-2.817714	-1.058274	-1.292702
11	6	0	0.465493	-0.523921	-0.587572
12	1	0	0.124325	-1.122556	0.256776
13	1	0	0.523028	-1.176460	-1.461644
14	1	0	-0.337086	1.055772	-1.666053
15	1	0	-2.783413	-1.380539	-0.362146
16	6	0	1.794785	0.143123	-0.304298
17	1	0	1.698725	0.814172	0.559114
18	1	0	2.079493	0.769276	-1.159830
19	6	0	2.883944	-0.886902	-0.031014
20	1	0	2.970486	-1.561038	-0.892715
21	1	0	2.583784	-1.514155	0.818090
22	6	0	4.230971	-0.238321	0.255690
23	1	0	5.005284	-0.986993	0.450281
24	1	0	4.566198	0.371047	-0.590593
25	1	0	4.177668	0.417270	1.131587

Butylcarbamate bu_cm_pd_water.log

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.112547	-1.760357	0.150545
2	1	0	-0.147925	-2.177045	1.070287
3	6	0	1.048614	-1.044716	-0.083503

4	8	0	2.034005	-1.271718	0.690146
5	8	0	1.071557	-0.243461	-1.068379
6	1	0	3.861249	1.094270	-1.369030
7	8	0	2.782177	1.248418	1.528977
8	1	0	2.955813	1.560285	0.621563
9	8	0	3.034075	1.557078	-1.207651
10	1	0	2.335777	0.857565	-1.193468
11	6	0	-1.389137	-1.320919	-0.385346
12	1	0	-1.268732	-1.145171	-1.456896
13	1	0	-2.093682	-2.152372	-0.284185
14	1	0	2.542301	0.313918	1.386658
15	6	0	-1.950945	-0.077160	0.292282
16	1	0	-2.088286	-0.280954	1.362991
17	1	0	-1.214541	0.733716	0.222329
18	6	0	-3.272027	0.369758	-0.321064
19	1	0	-3.127551	0.559040	-1.393118
20	1	0	-4.000618	-0.449386	-0.254576
21	6	0	-3.836008	1.615732	0.348905
22	1	0	-4.782990	1.928105	-0.103413
23	1	0	-4.021082	1.444204	1.415092
24	1	0	-3.139396	2.457617	0.269568