Supporting Information

NMR Speciation of Aqueous MAPA, Tertiary Amines, and Their Blends in the Presence of CO_2: Influence of pK_a and Reaction Mechanisms

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Content

Section S1: Densities

Densities (g/cm^3 and/or g/mL) of unloaded solutions were measured at 25°C using an Anton Paar DMA 4500M densitometer (0.01 kg/m^3 and 0.01 ºC nominal repeatability). The densities of the CO_2 loaded solutions were not measured using the same apparatus, but data equivalent to density are provided by weighing at room temperature 1 mL of sample (as measured by Hamilton syringes, model 1001 TLL) on a Mettler Toledo analytical balance (model ME204, d=0.0001g). The uncertainty in the measurements (< 0.6%) was calculated by comparing the weight of 1 mL of distilled water and pure MDEA (high viscous amine)[1], measured using the syringe, with the densities data at room temperature and at 293.15K.[2]

Table S1: Densities (g/cm^3 and/or g/mL) at 25°C of the unloaded solutions.

	Single Amine				MAPA:Tertiary Amine			
	0.5M	**1M**	**1.5M**	**3M**	**1M:3M**	**0.5M:1.5M**	**1M:1M**	**2M:2M**
MAPA	0.99438	0.99092	-	-	-	-	-	-
DEEA	-	-	0.99197	0.983	0.97551	0.98962	0.98892	0.97764
1DEA2P	-	-	0.98854	-	-	0.98562	0.98712	-
3DEA1P	-	-	0.98892	0.97484	0.98876	0.98648	0.98735	0.97224
Tropine	-	-	1.02153	-	-	1.01953	1.00892	-
EDEA	-	-	-	1.02796	1.02136	-	-	1.00793
BDEA	-	-	-	1.00142	0.99341	-	-	0.9894
t-BDEA	-	-	-	1.01559	1.006	-	-	0.99927
TEA	-	-	-	1.06432	1.05894	-	-	1.03264

Table S2: Densities (g/mL) of the solutions at room temperature after absorption experiments.

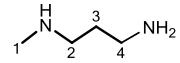
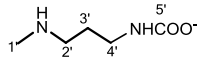
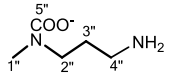
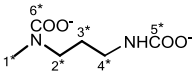
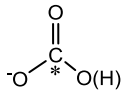
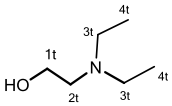
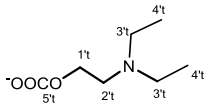
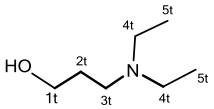
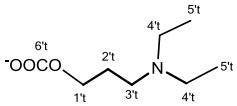
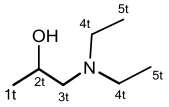
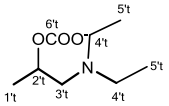
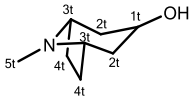
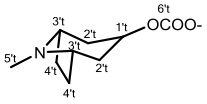
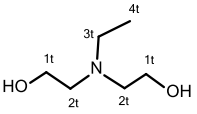
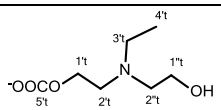
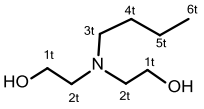
	Single Amine				MAPA:Tertiary Amine			
	0.5M	**1M**	**1.5M**	**3M**	**1M:3M**	**0.5M:1.5M**	**1M:1M**	**2M:2M**
MAPA	1.0149	1.034	-	-	-	-	-	-
DEEA	-	-	1.0391	1.0649	1.0862	1.0532	1.0554	1.0962
1DEA2P	-	-	1.0189	-	-	1.0568	1.0578	-
3DEA1P	-	-	1.0354	1.0467	1.0731	1.049	1.0522	1.098
Tropine	-	-	1.0732	-	-	1.0809	1.0804	-
EDEA	-	-	-	1.0397	1.0908	-	-	1.1133
BDEA	-	-	-	1.0098	1.0407	-	-	1.0768
t-BDEA	-	-	-	1.0327	1.0551	-	-	1.094
TEA	-	-	-	1.0681	1.1236	-	-	1.1134

Table S3: Densities (g/mL) of the solutions at room temperature after screening desorption experiments.

	Single Amine				MAPA:Tertiary Amine			
	0.5M	**1M**	**1.5M**	**3M**	**1M:3M**	**0.5M:1.5M**	**1M:1M**	**2M:2M**
MAPA	0.9998	1.0197	-	-	-	-	-	-
DEEA	-	-	1.0002	0.9855	0.9997	0.9975	1.0144	1.0075
1DEA2P	-	-	-	-	-	-	-	-
3DEA1P	-	-	0.9916	0.9726	0.9817	1.0056	1.0083	1.0155
Tropine	-	-	1.0628	-	-	1.041	1.0459	-
EDEA	-	-	-	1.0331	1.0424	-	-	1.0595
BDEA	-	-	-	0.9959	1.0053	-	-	1.0311
t-BDEA	-	-	-	1.0169	1.0287	-	-	1.0373
TEA	-	-	-	1.0701	1.0746	-	-	1.0736

Section S2: Signal assignment and chemical shift values

Table S4. Structure and numbering of the species in the solutions after both absorption and desorption screening tests.

Structure and carbons numbering	Name
	MAPA
	$MAPACOO^-_{(p)}$
	$MAPACOO^-_{(s)}$
	$MAPA(COO^-)_2$
	HCO_3^-/CO_3^{2-}
	DEEA
	$DEEAOCOO^-$
	3DEA1P
	$3DEA1POCOO^-$
	1DEA2P
	$1DEA2POCOO^-$
	TROPINE
	$TROPINEOCOO^-$
	EDEA
	$EDEAOCOO^-$
	BDEA

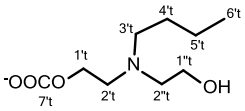
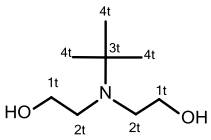
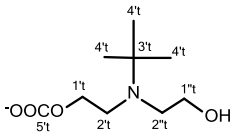
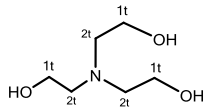
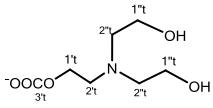
	BDEAOCOO$^-$
	*t*-BDEA
	*t*-BDEAOCOO$^-$
	TEA
	TEAOCOO$^-$

Table S5. Chemical shift values of the carbons belonging to the species in the blend 3M Tertiary amine/1M MAPA after absorption.[a]

3M Tertiary amine : 1M MAPA							
Absorption		**3DEA1P/MAPA**	**DEEA/MAPA**	**t-BDEA/MAPA**	**BDEA/MAPA**	**EDEA/MAPA**	**TEA/MAPA**
MAPA(H^+)$COO^-_{(p)}$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1'	33.4	33.3	33.3	33.4	33.3	33.2
	2'	47.1	47.0	47.0	47.1	47.0	47.0
	3'	27.6	27.4	27.3	27.4	27.4	27.3
	4'	38.5	38.4	38.3	38.4	38.3	38.2
	5'	164.7	164.8	164.7	164.9	164.8	164.8
MAPA(H^+)$COO^-_{(s)}$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1''	34.5	34.5	34.4	34.5	34.4	34.4
	2''	45.5	45.4	45.3	45.4	45.3	45.2
	3''	26.0	25.8	25.6	25.7	25.7	25.5
	4''	37.2	37.2	37.0	37.1	37.1	37.1
	5''	164.4	164.4	164.3	164.5	164.4	164.4
MAPA$(COO^-)_2$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1*	34.8	34.8	34.7	34.8	34.8	34.7
	2*	46.9	46.9	47.0	46.9	46.8	46.9
	3*	29.0	28.9	28.8	28.8	28.8	28.7
	4*	39.5	39.4	39.4	39.4	39.4	39.4
	5*	164.6	164.7	164.6	164.8	164.7	164.7
	6*	164.2	164.3	164.1	164.3	164.3	164.2
MAPA/MAPA$(H^+)_2$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1		33.6	33.6	33.7	33.6	33.5
	2			47.0		46.8	46.8
	3		25.8	25.7		25.9	25.5
	4		37.7	37.6	37.7	37.7	37.5
HCO_3^-/CO_3^{2-}	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	*	161.4	161.9	161.4	161.7	162.0	161.2
3° Amine/AmineH^+	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1 t	59.6	56.8	61.0	59.0	58.0	59.0
	2 t	27.1	53.9	52.9	56.2	55.0	56.3
	3 t	49.3	47.8	57.6	54.8	48.8	
	4 t	47.2	9.2	26.4	28.1	10.1	
	5 t	9.4			20.8		
	6 t				14.2		
3° Amine(H^+)$OCOO^-$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1't	63.5	61.4	65.1	63.1	62.5	63.3
	2' t	24.7	51.4	50.4	53.5	52.5	53.6
	3' t	49.2		57.4		48.8	159.3
	4' t		9.7			10.5	
	5' t	9.6	158.6	159.1		159.1	
	6' t	159.1					
	7' t				159.2		
	others					58.4 (1"t)	

Table S6. Chemical shift values of the carbons belonging to the species in the blend 3M Tertiary amine/1M MAPA after screening desorption.[a]

3M Tertiary amine : 1M MAPA							
Desorption		**3DEA1P/MAPA**	**DEEA/MAPA**	**t-BDEA/MAPA**	**BDEA/MAPA**	**EDEA/MAPA**	**TEA/MAPA**
MAPA(H^+)$COO^-_{(p)}$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1'	34.6	34.4	34.4	34.5	34.2	34.1
	2'	48.1	47.9	47.9	48.0	47.7	47.7
	3'	28.9	28.7	28.7	28.8	28.5	28.4
	4'	39.2	39.0	39.0	39.1	38.9	38.8
	5'	164.9	164.9	164.8	164.9	164.8	164.8
MAPA(H^+)$COO^-_{(s)}$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1''	34.6	34.6	34.5	34.6	34.5	34.5
	2''	46.0	45.9	45.8	45.9	45.8	45.7
	3''	28.5	28.1	28.1	28.1	27.8	27.7
	4''	38.1	37.9	37.8	37.9	37.8	37.8
	5''	164.5	164.5	164.3	164.5	164.4	164.4
MAPA(COO^-)$_2$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1*	34.8	34.8	34.7	34.8	34.8	34.8
	2*		46.9	46.8	46.9	46.9	46.8
	3*		28.8	28.7	28.8	28.8	28.8
	4*	39.5	39.5	39.4	39.4	39.4	39.4
	5*	164.9	164.9	164.7	164.9	164.8	164.7
	6*	164.4	164.4	164.3	164.4	164.3	164.3
MAPA/MAPA(H^+)$_2$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1	35.1	34.9	35.0	35.0	34.7	34.7
	2	48.6	48.4	48.5	48.5	48.3	48.2
	3	30.5	30.1	30.3	30.3	29.9	29.8
	4	39.2	39.1	39.1	39.1	39.0	38.9
HCO_3^-/CO_3^{2-}	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	*						
3° Amine/AmineH^+	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1 t	60.8	59.1	61.9	59.5	59.2	59.4
	2 t	28.9	54.4	52.8	56.3	55.3	56.4
	3 t	49.8	47.4	55.5	55.0	48.6	
	4 t	46.8	10.9	26.8	28.5	11.0	
	5 t	11.0			21.0		
	6 t				14.3		

Table S7. Chemical shift values of the carbons belonging to the species in the blend 2M Tertiary amine/2M MAPA after absorption.[a]

2M Tertiary amine : 2M MAPA							
Absorption		**3DEA1P/MAPA**	**DEEA/MAPA**	**t-BDEA/MAPA**	**BDEA/MAPA**	**EDEA/MAPA**	**TEA/MAPA**
MAPA(H^+)$COO^-_{(p)}$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1'	33.3	33.3	33.2	33.3	33.2	33.2
	2'	47.0	47.0	46.9	47.0	47.0	46.9
	3'	27.4	27.3	27.3	27.3	27.3	27.2
	4'	38.4	38.4	38.3	38.4	38.4	38.3
	5'	164.7	164.7	164.7	164.8	164.8	164.7
MAPA(H^+)$COO^-_{(s)}$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1''	34.4	34.4	34.4	34.5	34.4	34.4
	2''	45.4	45.4	45.3	45.4	45.3	45.3
	3''	25.7	25.7	25.6	25.7	25.6	25.6
	4''	37.2	37.2	37.1	37.1	37.1	37.1
	5''	164.3	164.4	164.3	164.4	164.4	164.4
MAPA(COO^-)$_2$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1*	34.8	34.8	34.7	34.7	34.7	34.7
	2*	46.8	46.8	46.8	46.8	46.8	46.5
	3*	28.9	28.8	28.8	28.8	28.7	28.7
	4*	39.4	39.4	39.4	39.4	39.4	39.4
	5*	164.6	164.7	164.6	164.7	164.7	164.7
	6*	164.2	164.2	164.1	164.3	164.2	164.2
MAPA/MAPA(H^+)$_2$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1	33.5	33.5	33.5	33.5	33.5	33.4
	2	46.7	46.7	46.6	46.7	46.6	46.6
	3	25.5	25.4	25.3	25.3	25.3	25.2
	4	37.5	37.5	37.4	37.5	37.4	37.4
HCO_3^-/CO_3^{2-}	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	*	161.3	161.7	161.4	161.7	161.8	161.4
3° Amine/AmineH^+	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1 t	59.2	56.4	60.1	58.6	57.5	58.8
	2 t	26.7	53.8	53.1	56.0	54.9	56.3
	3 t	49.2	47.8	59.3	54.7	48.9	
	4 t	47.3	8.9	25.6	27.9	9.7	
	5 t	9.0			20.7		
	6 t				14.1		
3° Amine(H^+)$OCOO^-$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1't	63.1	60.9	64.6	62.9	62.2	63.2
	2' t	24.2	51.3	50.6	53.4	52.5	53.6
	3' t	49.2		58.4			159.3
	4' t		9.4	26.0			
	5' t	9.0	158.5	159.0		159.0	
	6' t	159.0					
	7' t				159.1		
	others						

Table S8. Chemical shift values of the carbons belonging to the species in the blend 2M Tertiary amine/2M MAPA after screening desorption.[a]

2M Tertiary amine : 2M MAPA							
Desorption		**3DEA1P/MAPA**	**DEEA/MAPA**	**t-BDEA/MAPA**	**BDEA/MAPA**	**EDEA/MAPA**	**TEA/MAPA**
$MAPA(H^+)COO^-_{(p)}$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1'	34.4	34.2	34.2	34.3	34.1	34.1
	2'	47.9	47.7	47.7	47.8	47.6	47.6
	3'	28.7	28.4	28.5	28.5	28.3	28.3
	4'	39.1	38.9	38.9	39.0	38.8	38.8
	5'	164.9	164.8	164.7	164.8	164.8	164.7
$MAPA(H^+)COO^-_{(s)}$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1''	34.6	34.5	34.5	34.5	34.5	34.5
	2''	46.0	45.8	45.8	45.9	45.8	45.8
	3''	28.2	27.8	28.0	27.9	27.6	27.7
	4''	38.0	37.8	37.8	37.8	37.7	37.7
	5''	164.4	164.4	164.3	164.4	164.4	164.4
$MAPA(COO^-)_2$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1*	34.8	34.8	34.7	34.7	34.8	34.7
	2*	46.9	46.9	46.8	46.8	46.8	46.8
	3*	28.9	28.8	28.7	28.8	28.8	28.7
	4*	39.5	39.4	39.4	39.4	39.4	39.4
	5*	164.8	164.8	164.7	164.8	164.7	164.7
	6*	164.4	164.3	164.2	164.3	164.3	164.3
$MAPA/MAPA(H^+)_2$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1	34.8	34.6	34.7	34.7	34.5	34.5
	2	48.3	48.2	48.2	48.3	48.1	48.0
	3	30.0	29.5	29.8	29.8	29.4	29.4
	4	39.0	38.9	38.9	38.9	38.8	38.8
HCO_3^-/CO_3^{2-}	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	*						
3° Amine/$AmineH^+$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1 t	60.6	58.9	61.8	59.4	59.2	59.4
	2 t	28.7	54.2	52.7	56.3	55.3	56.4
	3 t	49.6	47.4	55.6	54.9	48.6	
	4 t	46.8	10.7	26.8	28.5	10.9	
	5 t	10.8			20.9		
	6 t				14.3		

Table S9. Chemical shift values of the carbons belonging to the species in the blend 1.5M Tertiary amine/0.5M MAPA after absorption.[a]

1.5 M Tertiary amine : 0.5 M MAPA					
Absorption		**Tropine/MAPA**	**DEEA/MAPA**	**3DEA1P/MAPA**	**1DEA2P/MAPA**
MAPA(H^+)$COO^-_{(p)}$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**
	1'	33.3	33.4	33.4	33.3
	2'	47.1	47.1	47.1	47.1
	3'	27.3	27.3	27.3	27.3
	4'	38.4	38.4	38.4	38.3
	5'	164.9	165.0	165.0	165.0
MAPA(H^+)$COO^-_{(s)}$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**
	1''	34.4	34.4	34.4	34.4
	2''	45.4	45.4	45.4	45.3
	3''	25.6	25.6	25.6	25.5
	4''	37.3	37.3	37.3	37.2
	5''	164.6	164.6	164.6	164.6
MAPA(COO^-)$_2$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**
	1*	34.8	34.8	34.8	34.8
	2*	46.9	46.9	46.9	46.9
	3*	28.7	28.7	28.7	28.7
	4*	39.5	39.5	39.5	39.4
	5*	164.9	165.0	164.9	164.9
	6*	164.4	164.5	164.4	164.4
MAPA/MAPA(H^+)$_2$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**
	1		33.6	33.6	33.6
	2				
	3		25.5		
	4		37.6	37.7	37.6
HCO_3^-/CO_3^{2-}	**Number**	**ppm**	**ppm**	**ppm**	**ppm**
	*	161.7	161.9	161.4	161.8
3° Amine/AmineH^+	**Number**	**ppm**	**ppm**	**ppm**	**ppm**
	1 t	61.9	56.3	59.3	20.9
	2 t	37.3	53.9	26.6	62.4
	3 t	63.0	47.9	49.5	58.7
	4 t	24.2	8.8	47.7	48.3
	5 t	39.2		8.9	8.7
3° Amine(H^+)$OCOO^-$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**
	1't	65.7	60.7	63.2	18.6
	2' t	35.7	51.6	24.1	67.2
	3' t		48.2	49.3	
	4' t		9.1		
	5' t		158.7		
	6' t	158.9		159.3	158.3
	7' t				
	others				

Table S10. Chemical shift values of the carbons belonging to the species in the blend 1.5M Tertiary amine/0.5M MAPA after screening desorption.[a]

1.5 M Tertiary amine : 0.5 M MAPA				
Desorption		**Tropine/MAPA**	**DEEA/MAPA**	**3DEA1P/MAPA**
MAPA(H^+)$COO^-_{(p)}$	**Number**	**ppm**	**ppm**	**ppm**
	1'	34.3	34.3	34.4
	2'	47.9	47.9	48.0
	3'	28.6	28.6	28.8
	4'	39.1	39.0	39.1
	5'	165.0	165.1	165.0
MAPA(H^+)$COO^-_{(s)}$	**Number**	**ppm**	**ppm**	**ppm**
	1''	34.5	34.5	34.6
	2''	46.0	46.0	46.1
	3''	28.4	28.2	28.5
	4''	38.1	38.0	38.1
	5''	164.5	164.6	164.6
MAPA(COO^-)$_2$	**Number**	**ppm**	**ppm**	**ppm**
	1*	34.8	34.8	34.8
	2*	46.9	47.4	47.0
	3*	28.7	28.7	28.7
	4*	39.5	39.5	39.5
	5*	164.9	165.0	165.0
	6*	164.5	164.5	164.5
MAPA/MAPA(H^+)$_2$	**Number**	**ppm**	**ppm**	**ppm**
	1	34.6	34.7	34.7
	2	48.2	48.3	48.3
	3	29.9	30.2	30.4
	4		39.0	39.0
HCO_3^-/CO_3^{2-}	**Number**	**ppm**	**ppm**	**ppm**
	*	166.9		
3° Amine/AmineH^+	**Number**	**ppm**	**ppm**	**ppm**
	1 t	63.2	59.0	60.7
	2 t	38.6	53.9	28.2
	3 t	61.5	47.4	49.3
	4 t	24.9	10.6	46.8
	5 t	40.1		10.5

Table S11. Chemical shift values of the carbons belonging to the species in the blend 1M Tertiary amine/1M MAPA after absorption.[a]

1 M Tertiary amine : 1 M MAPA					
Absorption		**Tropine/MAPA**	**DEEA/MAPA**	**3DEA1P/MAPA**	**1DEA2P/MAPA**
$MAPA(H^+)COO^-_{(p)}$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**
	1'	33.3	33.3	33.3	33.3
	2'	47.1	47.1	47.1	47.1
	3'	27.2	27.3	27.3	27.2
	4'	38.3	38.3	38.3	38.3
	5'	165.0	165.0	165.0	165.0
$MAPA(H^+)COO^-_{(s)}$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**
	1''	34.4	34.4	34.4	34.4
	2''	45.3	45.3	45.3	45.3
	3''	25.5	25.5	25.6	25.5
	4''	37.3	37.3	37.3	37.2
	5''	164.6	164.6	164.6	164.6
$MAPA(COO^-)_2$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**
	1*	34.7	34.8	34.8	34.8
	2*	46.9	46.9	46.9	46.9
	3*	28.7	28.7	28.7	28.6
	4*	39.4	39.5	39.5	39.4
	5*	164.9	165.0	164.9	164.9
	6*	164.4	164.5	164.4	164.5
$MAPA/MAPA(H^+)_2$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**
	1	33.5	33.5	33.5	33.5
	2	46.7	46.7	46.8	46.7
	3	25.3	25.3	25.3	25.3
	4		37.5	37.5	37.5
HCO_3^-/CO_3^{2-}	**Number**	**ppm**	**ppm**	**ppm**	**ppm**
	1	161.6	161.8	161.4	161.6
3° Amine/$AmineH^+$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**
	1 t	61.9	56.2	59.3	20.8
	2 t	37.3	53.8	26.5	62.4
	3 t	63.0	47.9	49.5	58.6
	4 t	24.1	8.7	47.7	48.3
	5 t	39.1		8.8	8.6
3° $Amine(H^+)OCOO^-$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**
	1't	65.6	60.6	63.2	
	2' t	35.7	51.6	24.1	
	3' t		48.3	49.3	
	4' t		9.0		
	5' t		158.6		
	6' t	158.9		159.4	
	7' t				
	others				

Table S12. Chemical shift values of the carbons belonging to the species in the blend 1M Tertiary amine/1M MAPA after screening desorption.[a]

1 M Tertiary amine : 1 M MAPA				
Desorption		**Tropine/MAPA**	**DEEA/MAPA**	**3DEA1P/MAPA**
MAPA(H^+)$COO^-_{(p)}$	**Number**	**ppm**	**ppm**	**ppm**
	1'	34.3	34.1	34.3
	2'	47.8	47.7	47.9
	3'	28.5	28.4	28.6
	4'	39.0	38.9	39.0
	5'	165.0	165.0	165.0
MAPA(H^+)$COO^-_{(s)}$	**Number**	**ppm**	**ppm**	**ppm**
	1''	34.5	34.5	34.5
	2''	46.0	45.9	46.0
	3''	28.2	27.9	28.3
	4''	38.0	37.9	38.1
	5''	164.6	164.6	164.6
MAPA(COO^-)$_2$	**Number**	**ppm**	**ppm**	**ppm**
	1*	34.8	34.8	34.8
	2*	46.9	46.9	46.8
	3*	28.6	28.7	28.7
	4*	39.5	39.5	39.5
	5*	164.9	165.0	165.0
	6*	164.5	164.5	164.5
MAPA/MAPA(H^+)$_2$	**Number**	**ppm**	**ppm**	**ppm**
	1	34.6	34.5	34.6
	2	48.2	48.1	48.2
	3	29.9	29.7	30.1
	4	38.9	38.8	38.9
HCO_3^-/CO_3^{2-}	**Number**	**ppm**	**ppm**	**ppm**
	*	166.9		
3° Amine/AmineH^+	**Number**	**ppm**	**ppm**	**ppm**
	1 t	63.1	58.8	60.6
	2 t	38.5	53.8	28.1
	3 t	61.5	47.4	49.2
	4 t	24.8	10.4	46.8
	5 t	40.0		10.4

Table S13. Chemical shift values of the carbons belonging to the species in 1.5M Tertiary amine after absorption.[a]

1.5 M Tertiary amine					
Absorption		**Tropine**	**DEEA**	**3DEA1P**	**1DEA2P**
HCO_3^-/CO_3^{2-}	**Number**	**ppm**	**ppm**	**ppm**	**ppm**
	*	162.6	162.3	161.5	162.2
3° Amine/AmineH^+	**Number**	**ppm**	**ppm**	**ppm**	**ppm**
	1 t	62.0	56.4	59.4	20.8
	2 t	37.4	53.9	26.6	62.5
	3 t	62.9	47.9	49.5	58.7
	4 t	24.2	8.8	47.7	48.3
	5 t	39.2		8.9	8.7
3° Amine(H^+)$OCOO^-$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**
	1't	65.8	60.9	63.3	
	2' t	35.8	51.6	24.2	67.4
	3' t	62.7	48.2	49.4	
	4' t		9.2		
	5' t		158.8		
	6' t	159.0		159.4	158.4
	7' t				
	others				

Table S14. Chemical shift values of the carbons belonging to the species in 1.5M Tertiary amine after screening desorption.[a]

1.5 M Tertiary amine				
Desorption		**Tropine**	**DEEA**	**3DEA1P**
HCO_3^-/CO_3^{2-}	**Number**	**ppm**	**ppm**	**ppm**
	*	165.6	166.0	166.0
3° Amine/AmineH^+	**Number**	**ppm**	**ppm**	**ppm**
	1 t	62.5	58.6	60.6
	2 t	37.8	53.9	28.0
	3 t	62.3	47.5	49.3
	4 t	24.4	10.3	46.9
	5 t	39.5		10.3

Table S15. Chemical shift values of the carbons belonging to the species in 3 M Tertiary amine after absorption.[a]

3M Tertiary amine							
Absorption		**3DEA1P**	**DEEA**	**t-BDEA**	**BDEA**	**EDEA**	**TEA**
HCO_3^-/CO_3^{2-}	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	*	161.9	162.5	161.5	161.7	162.5	160.9
3° Amine/AmineH^+	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1 t	59.8	56.8	61.2	59.1	58.7	59.3
	2 t	27.3	54.0	52.8	56.1	55.1	56.3
	3 t	49.4	47.8	57.2	54.8	48.7	
	4 t	47.2	9.2	26.4	28.1	10.5	
	5 t	9.6			20.9		
	6 t				14.2		
3° Amine(H^+)$OCOO^-$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1't	63.7	61.4	65.2	63.1	62.9	63.4
	2' t	24.9	51.4	50.4	53.4	52.5	53.5
	3' t	49.2	47.8	57.4			159.4
	4' t		9.7			10.7	
	5' t		158.7	159.2		159.3	
	6' t	159.3					
	7' t				159.4		
	others						

Table S16. Chemical shift values of the carbons belonging to the species in 3 M Tertiary amine after screening desorption.[a]

3M Tertiary amine							
Desorption		**3DEA1P**	**DEEA**	**t-BDEA**	**BDEA**	**EDEA**	**TEA**
HCO_3^-/CO_3^{2-}	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	*	164.9	165.3	162.2	162.3	162.8	161.0
3° Amine/AmineH^+	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1 t	60.9	59.1	61.8	59.4	59.1	59.4
	2 t	28.7	54.2	52.6	56.2	55.2	56.3
	3 t	49.7	47.4	55.9	54.9	48.6	
	4 t	46.9	10.7	26.7	28.4	10.8	
	5 t	10.8			21.0		
	6 t				14.3		
3° Amine(H^+)$OCOO^-$	**Number**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**	**ppm**
	1't		63.1	65.7	63.4	63.2	63.5
	2' t		51.4			52.5	53.5
	3' t						159.4
	4' t			50.1			
	5' t		159.4	159.3		159.4	
	6' t	159.6					
	7' t				159.4		
	others						

Table S17. Chemical shift values of the carbons belonging to the species in single MAPA after a) absorption and b) screening desorption.[a]

a) Absorption		MAPA 1M	MAPA 0.5M
$MAPA(H^+)COO^-_{(p)}$	Number	ppm	ppm
	1'	33.3	33.4
	2'	47.2	47.2
	3'	27.2	27.3
	4'	38.3	38.3
	5'	165.1	165.2
$MAPA(H^+)COO^-_{(s)}$	Number	ppm	ppm
	1''	34.4	34.4
	2''	45.3	45.3
	3''	25.5	25.4
	4''	37.3	37.3
	5''	164.8	164.8
$MAPA(COO^-)_2$	Number	ppm	ppm
	1*	34.8	
	2*	46.9	
	3*	28.6	
	4*	39.5	
	5*		
	6*	164.6	
$MAPA/MAPA(H^+)_2$	Number	ppm	ppm
	1	33.5	33.6
	2	46.7	46.8
	3	25.1	25.1
	4	37.5	37.6
HCO_3^-/CO_3^{2-}	Number	ppm	ppm
	*	161.5	161.0

b) Desorption		MAPA 1M	MAPA 0.5M
$MAPA(H^+)COO^-_{(p)}$	Number	ppm	ppm
	1'	33.7	34.1
	2'	47.4	47.7
	3'	27.7	28.2
	4'	38.6	38.8
	5'	165.2	165.2
$MAPA(H^+)COO^-_{(s)}$	Number	ppm	ppm
	1''	34.5	34.5
	2''	45.6	45.9
	3''	26.6	27.7
	4''	37.6	37.9
	5''	164.7	164.8
$MAPA(COO^-)_2$	Number	ppm	ppm
	1*	34.8	34.8
	2*	46.9	47.0
	3*	28.6	28.6
	4*	39.5	39.5
	5*	165.1	165.2
	6*	164.6	164.7
$MAPA/MAPA(H^+)_2$	Number	ppm	ppm
	1	34.1	34.3
	2	47.8	48.1
	3	28.5	29.6
	4	38.6	38.7
HCO_3^-/CO_3^{2-}	Number	ppm	ppm
	*	166.2	

Section S3: Speciations

The concentrations (mol/L) of all the species found in each amine systems after both absorption and desorption on the screening apparatus are reported in table S18-S31. The term "traces" is used when the species was found in quantity lower than 0.01 mol/L and/or the signals were broadened with baseline.

Table S18. Concentration (mol/L) of the species in the blend 3M tertiary amine/1M MAPA after absorption.

	3M tertiary amine : 1M MAPA					
Absorption	**3DEA1P/MAPA**	**DEEA/MAPA**	**t-BDEA/MAPA**	**BDEA/MAPA**	**EDEA/MAPA**	**TEA/MAPA**
MAPA(H^+)$COO^-_{(p)}$	0.394	0.456	0.578	0.611	0.575	0.642
MAPA(COO^-)$_2$	0.482	0.399	0.149	0.120	0.212	0.066
MAPA(H^+)$COO^-_{(s)}$	0.112	0.119	0.174	0.190	0.160	0.185
MAPA/MAPA(H^+)$_2$	---	0.020	0.064	0.087	0.046	0.107
HCO_3^-/CO_3^{2-}	1.06	1.33	0.306	0.266	0.571	0.262
3° Amine(H^+)$OCOO^-$	0.096	0.064	0.071	0.059	0.104	0.086
3° Amine/AmineH^+	2.92	2.95	2.94	2.96	2.93	2.96

Table S19. Concentration (mol/L) of the species in the blend 3M tertiary amine/1M MAPA after screening desorption.

	3M tertiary amine : 1M MAPA					
Desorption	**3DEA1P/MAPA**	**DEEA/MAPA**	**t-BDEA/MAPA**	**BDEA/MAPA**	**EDEA/MAPA**	**TEA/MAPA**
MAPA(H^+)$COO^-_{(p)}$	0.375	0.401	0.303	0.302	0.386	0.371
MAPA(COO^-)$_2$	0.042	0.052	0.022	0.022	0.036	0.030
MAPA(H^+)$COO^-_{(s)}$	0.116	0.123	0.095	0.097	0.120	0.111
MAPA/MAPA(H^+)$_2$	0.483	0.381	0.510	0.506	0.453	0.475
HCO_3^-/CO_3^{2-}	---	---	---	---	---	---
3° Amine(H^+)$OCOO^-$	---	traces	traces	traces	traces	traces
3° Amine/AmineH^+	3.05	2.93	2.92	2.82	3.03	3.08

Table S20. Concentration (mol/L) of the species in the blend 2M tertiary amine/2M MAPA after absorption.

	2M tertiary amine : 2M MAPA					
Absorption	**3DEA1P/MAPA**	**DEEA/MAPA**	**t-BDEA/MAPA**	**BDEA/MAPA**	**EDEA/MAPA**	**TEA/MAPA**
MAPA(H^+)$COO^-_{(p)}$	1.19	1.14	1.27	1.28	1.21	1.28
MAPA(COO^-)$_2$	0.531	0.416	0.264	0.209	0.275	0.141
MAPA(H^+)$COO^-_{(s)}$	0.313	0.288	0.371	0.373	0.321	0.348
MAPA/MAPA(H^+)$_2$	0.090	0.092	0.186	0.223	0.140	0.245
HCO_3^-/CO_3^{2-}	0.912	0.879	0.450	0.373	0.583	0.369
3° Amine(H^+)$OCOO^-$	0.049	0.027	0.053	0.043	0.053	0.064
3° Amine/AmineH^+	2.06	1.94	2.08	2.02	1.93	1.99

Table S21. Concentration (mol/L) of the species in the blend 2M tertiary amine/2M MAPA after screening desorption.

	2M tertiary amine : 2M MAPA					
Desorption	**3DEA1P/MAPA**	**DEEA/MAPA**	**t-BDEA/MAPA**	**BDEA/MAPA**	**EDEA/MAPA**	**TEA/MAPA**
$MAPA(H^+)COO^-_{(p)}$	0.774	0.898	0.741	0.794	0.819	0.833
$MAPA(COO^-)_2$	0.101	0.126	0.077	0.082	0.092	0.088
$MAPA(H^+)COO^-_{(s)}$	0.245	0.267	0.227	0.243	0.244	0.248
$MAPA/MAPA(H^+)_2$	0.920	0.849	1.02	1.01	0.854	0.953
HCO_3^-/CO_3^{2-}	---	---	---	---	---	---
3° $Amine(H^+)OCOO^-$	---	---	traces	---	traces	traces
3° $Amine/AmineH^+$	2.04	2.12	2.12	2.16	2.05	2.12

Table S22. Concentration (mol/L) of the species in the blend 1.5M tertiary amine/0.5M MAPA after absorption.

	1.5M tertiary amine : 0.5M MAPA			
Absorption	**MAPA/TROPINE**	**3DEA1P/MAPA**	**1DEA2P/MAPA**	**MAPA/DEEA**
$MAPA(H^+)COO^-_{(p)}$	0.318	0.321	0.314	0.314
$MAPA(COO^-)_2$	0.097	0.101	0.084	0.078
$MAPA(H^+)COO^-_{(s)}$	0.068	0.073	0.067	0.066
$MAPA/MAPA(H^+)_2$	---	0.022	0.021	0.024
HCO_3^-/CO_3^{2-}	1.18	1.16	1.09	1.08
3° $Amine(H^+)OCOO^-$	0.044	0.044	traces (0.008)	0.024
3° $Amine/AmineH^+$	1.36	1.53	1.42	1.44

Table S23. Concentration (mol/L) of the species in the blend 1.5M tertiary amine/0.5M MAPA after screening desorption.

	1.5M tertiary amine : 0.5M MAPA			
Desorption	**MAPA/TROPINE**	**3DEA1P/MAPA**	**1DEA2P/MAPA**	**MAPA/DEEA**
$MAPA(H^+)COO^-_{(p)}$	0.250	0.225	n.a.	0.225
$MAPA(COO^-)_2$	0.078	0.031	n.a.	0.024
$MAPA(H^+)COO^-_{(s)}$	0.064	0.063	n.a.	0.060
$MAPA/MAPA(H^+)_2$	0.115	0.206	n.a.	0.230
HCO_3^-/CO_3^{2-}	0.193	---	n.a.	---
3° $Amine(H^+)OCOO^-$	traces	---	n.a.	---
3° $Amine/AmineH^+$	1.43	1.56	n.a.	1.61

Table S24. Concentration (mol/L) of the species in the blend 1M tertiary amine/1M MAPA after absorption.

	1M tertiary amine : 1M MAPA			
Absorption	**MAPA/TROPINE**	**3DEA1P/MAPA**	**1DEA2P/MAPA**	**MAPA/DEEA**
$MAPA(H^+)COO^-_{(p)}$	0.673	0.647	0.685	0.665
$MAPA(COO^-)_2$	0.107	0.102	0.095	0.090
$MAPA(H^+)COO^-_{(s)}$	0.146	0.140	0.149	0.143
$MAPA/MAPA(H^+)_2$	0.072	0.070	0.078	0.075
HCO_3^-/CO_3^{2-}	0.806	0.779	0.791	0.780
$Amine(H^+)OCOO^-$	0.020	0.020	traces	0.012
3° $Amine/AmineH^+$	0.912	0.949	0.948	0.993

Table S25. Concentration (mol/L) of the species in the blend 1M tertiary amine/1M MAPA after screening desorption.

	1M tertiary amine : 1M MAPA			
Desorption	**MAPA/TROPINE**	**3DEA1P/MAPA**	**1DEA2P/MAPA**	**MAPA/DEEA**
$MAPA(H^+)COO^-_{(p)}$	0.475	0.387	n.a.	0.437
$MAPA(COO^-)_2$	0.078	0.041	n.a.	0.044
$MAPA(H^+)COO^-_{(s)}$	0.130	0.105	n.a.	0.114
$MAPA/MAPA(H^+)_2$	0.365	0.458	n.a.	0.456
HCO_3^-/CO_3^{2-}	0.149	---	n.a.	---
3° $Amine(H^+)OCOO^-$	---	---	n.a.	---
3° $Amine/AmineH^+$	0.972	0.970	n.a.	1.028

Table S26. Concentration (mol/L) of the species in single tertiary amine 3M after absorption.

	3M tertiary amine					
Absorption	**3DEA1P**	**DEEA**	**t-BDEA**	**BDEA**	**EDEA**	**TEA**
HCO_3^-/CO_3^{2-}	1.66	1.90	0.357	0.210	0.389	0.120
3° $Amine(H^+)OCOO^-$	0.134	0.085	0.096	0.051	0.078	0.050
3° $Amine/AmineH^+$	3.01	2.97	3.20	2.75	2.97	3.04

Table S27. Concentration (mol/L) of the species in single tertiary amine 3M after screening desorption.

	3M tertiary amine					
Desorption	**3DEA1P**	**DEEA**	**t-BDEA**	**BDEA**	**EDEA**	**TEA**
HCO_3^-/CO_3^{2-}	0.127	0.166	0.045	0.037	0.133	0.068
3° $Amine(H^+)OCOO^-$	traces	0.010	0.011	traces (0.007)	0.024	0.024
3° $Amine/AmineH^+$	3.17	2.94	3.11	3.11	3.09	3.09

Table S28. Concentration (mol/L) of the species in single tertiary amine 1.5M after absorption.

	1.5M tertiary amine			
Absorption	**TROPINE**	**3DEA1P**	**1DEA2P**	**DEEA**
HCO_3^-/CO_3^{2-}	1.23	1.18	1.18	1.13
3° Amine(H^+)$OCOO^-$	0.048	0.045	traces (0.008)	0.027
3° Amine/AmineH^+	1.39	1.46	1.45	1.50

Table S29. Concentration (mol/L) of the species in single tertiary amine 1.5M after screening desorption.

	1.5M tertiary amine			
Desorption	**TROPINE**	**3DEA1P**	**1DEA2P**	**DEEA**
HCO_3^-/CO_3^{2-}	0.740	0.220	n.a.	0.222
3° Amine(H^+)$OCOO^-$	traces	traces	n.a.	traces
3° Amine/AmineH^+	1.47	1.55	n.a.	1.52

Table S30. Concentration (mol/L) of the species in single MAPA 1M and 0.5M after absorption.

Absorption	**MAPA 1M**	**MAPA 0.5 M**
MAPA(H^+)$COO^-_{(p)}$	0.657	0.293
MAPA$(COO^-)_2$	0.019	----
MAPA(H^+)$COO^-_{(s)}$	0.140	0.064
MAPA/MAPA$(H^+)_2$	0.218	0.119
HCO_3^-/CO_3^{2-}	0.310	0.116

Table S31. Concentration (mol/L) of the species in single MAPA 1M and 0.5M after screening desorption.

Desorption	**MAPA 1M**	**MAPA 0.5 M**
MAPA(H^+)$COO^-_{(p)}$	0.503	0.172
MAPA$(COO^-)_2$	0.035	traces (0.008)
MAPA(H^+)$COO^-_{(s)}$	0.117	0.041
MAPA/MAPA$(H^+)_2$	0.347	0.293
HCO_3^-/CO_3^{2-}	0.086	---

References

(1) Pinto, D. D. D.; Johnsen, B.; Awais, M.; Svendsen, H. F.; Knuutila, H. K., Viscosity measurements and modeling of loaded and unloaded aqueous solutions of MDEA, DMEA, DEEA and MAPA. *Chemical Engineering Science* **2017,** 171, (Supplement C), 340-350.
(2) Pinto, D. D. D.; Monteiro, J. G. M. S.; Johnsen, B.; Svendsen, H. F.; Knuutila, H., Density measurements and modelling of loaded and unloaded aqueous solutions of MDEA (N-methyldiethanolamine), DMEA (N,N-dimethylethanolamine), DEEA (diethylethanolamine) and MAPA (N-methyl-1,3-diaminopropane). *International Journal of Greenhouse Gas Control* **2014,** 25, 173-185.

Footnotes

[a] All the chemical shift values (Table S5-S17) are reported using as reference the peak of the methyl carbon of acetonitrile (internal reference standard) which resonates at 1.47 ppm.