Supporting information

Table 1: Deformation and coordination energies (kJ/mol) of ammonia-water clusters at the MP2/6-311+G(2d,2p) computational level.

n		E_{def}	$\mathbf{\Delta E_{coord}}$
1	**1-I**	0.46	-24.93
2	**1-II**	2.01	-59.98
3	**1-III-cyc-ext**	2.67	-86.69
3	**1- III-cyc**	4.67	-98.97
4	**1-IV-cyc-ext**	5.74	-130.5
4	**1-IV-cyc**	6.72	-131.5
4	**1-IV-prot**	757.23	-60.89
5	**1-Vcyc-ext**	7.51	-161.66
5	**1-V-cyc**	8.26	-158.66
5	**1-V-prot**	699.66	-102.59
6	**1-VI-cyc**	10.23	-114.23
6	**1-VI-cyc-ext**	25.52	-134.24
6	**1-VI-prot**	1356.68	-42.29
7	**1-VII-cyc-ext**	28.49	-158.8
7	**1-VII-prot**	1460.63	-86.1613

Table 2: Deformation and coordination energies (kJ/mol) of methylamine-water clusters at the MP2/6-311+G(2d,2p) computational level.

n		E_{def}	ΔE_{coord}
1	**2-I**	0.85	-27.87
2	**2-II**	2.86	-62.54
3	**2-III-cyc-ext**	5.96	-99.36
3	**2-III-cyc**	6.16	-101.97
4	**2-IV-cyc-ext**	6.43	-133.56
4	**2-IV-cyc**	8.70	-134.31
4	**2-IV-prot**	767.47	-79.05
4	**2-IV-prot-met**	648.26	-60.96
5	**2-V-cyc-ext**	8.69	-165.50
5	**2-V-cyc**	10.15	-161.35
5	**2-V-prot**	1180.10	-114.21
5	**2-V-prot-met1**	972.60	-74.02
5	**2-V-prot-met2**	582.63	-111.00
6	**2-VI-cyc**	…	…
6	**2-VI-cyc-ext**	…	…
6	**2-VI-prot**	1364.61	-61.82
6	**2-VI-prot-met**	790.97	-41.47
7	**2-VII-cyc-ext**	…	…
7	**2-VII-prot**	1471.72	-105.80

Table 3: Deformation and coordination energies (kJ/mol) of dimethylamine-water clusters at the MP2/6-311+G(2d,2p) computational level.

n		E_{def}	ΔE_{coord}
1	**3-I**	0.97	-29.35
2	**3-II**	3.24	-63.64
3	**3-III-cyc-ext**	4.21	-106.35
3	**3-III-cyc**	7.04	-90.84
3	**3-III-cyc-met**	5.92	-95.47
4	**3-IV-cyc-ext**	6.98	-134.86
4	**3-IV-cyc**	9.62	-136.56
4	**3-IV-cyc-met**	7.49	-124.86
4	**3-IV-prot-met**	663.73	-85.44
5	**3-V-cyc-ext**	9.18	-167.92
5	**3-V-cyc**	12.66	-164.52
5	**3-V-prot-met1**	981.91	-96.59
5	**3-V-prot-met2**	596.29	-132.66
6	**3-VI-cyc**	···	···
6	**3-VI-cyc-ext**	···	···
6	**3-VI-Prot-met**	1508.60	-50.73
7	**3-VII-cyc-ext**	···	···
7	**3-VII-prot-met**	782.07	-77.19

Table 4: Deformation and coordination energies (kJ/mol) of trimethylamine-water clusters at the MP2/6-311+G(2d,2p) computational level.

n		E_{def}	ΔE_{coord}
1	**4-I**	1.15	-29.16
2	**4-II-cyc-ext**	3.85	-63.13
3	**4-III-cyc-ext**	5.03	-93.65
3	**4-III-cyc-met**	6.56	-96.04
4	**4-IV-cyc-ext**	7.60	-136.77
4	**4-IV-cyc-met**	8.11	-125.59
5	**4-V-cyc-ext**	9.39	-168.84
6	**4-VI-cyc-ext**	···	···
7	**4-VII-cyc-ext**	···	···

Table 5: Vibration modes (cm^{-1}) associated with the stretching frequency of the closest O-H bond to the amino group obtained at the MP2/6-311+G(2d,2p) computational level.

n	*Cyc*	*Cyc-ext*
Ammonia		
1	3612	…
2	3434	…
3	3261	3549
4	3197	3545
5	3165	3559
6	3598	3553
7	…	3547
Methylamine		
1	3543	…
2	3333	…
3	3128	3134
4	3042	3279
5	3012	3458
6	…	…
7	…	…
Dimethylamine		
1	3486	…
2	3255	…
3	3042	3302
4	2926	3386
5	2866	3380
6	…	…
7	…	…
Trimethylamine		
1	3443	…
2	3168	…
3	3459	3199
4	3030	3328
5	…	3334
6	…	…
7	…	…

Table 6: Vibration modes (cm^{-1}) associated with the stretching frequency of the longest N-H bond obtained at the MP2/6-311+G(2d,2p) computational level.

n	*Cyc*	*Prot (sym)*	*Prot (asym)*
Ammonia			
1	3634	⋯	⋯
2	3601	⋯	⋯
3	3582	⋯	⋯
4	3421	3045	3054/3055
5	3409	⋯	2912
6	3473	⋯	2911
7	⋯	2992	2970/2970
Methylamine			
1	3543	⋯	⋯
2	3494	⋯	⋯
3	3465	⋯	⋯
4	3440	2573	2768/2798
5	3421	⋯	2963
6	⋯	⋯	2947
7	⋯	3041	3029/3029
Dimethylamine			
1	3545	⋯	⋯
2	3498	⋯	⋯
3	3466	⋯	⋯
4	3438	2862	2846
5	3430	⋯	2752/2804
6	⋯	⋯	2978
7	⋯	⋯	2399