Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information 1 for

From Bonds to Interactions: Comprehensive Molecular Characterization via Polarizable Bond-Dipole Approach

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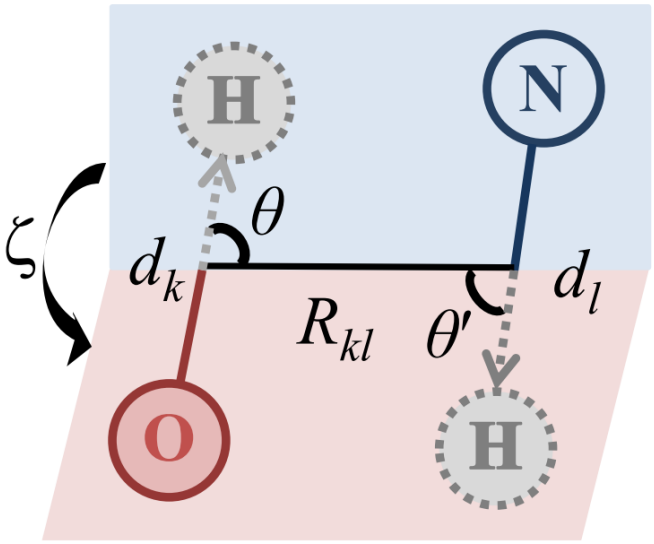

Fig. S1 The diagrammatic sketch of dipole-dipole interaction

Table S1 Parameters utilized in this work

Parameters for bond stretching		
bond[a]	b_{eq} (Å)	Bond force constant (K_b, kcal·mol^{-1}·Å^{-2})
O-H in water	0.9572	605.0
O-H in methanol	0.9611	596.0
C-H in methanol	1.0859	365.0
C-O in methanol	1.4237	425.0
N-H in methylamine	1.0120	510.0
C-H in methylamine	1.0901	385.0
C-N in methylamine	1.4634	385.0
C=O in NMA	1.2246	605.0
N-H in NMA	1.0090	534.0
N-C in NMA	1.3689	404.0
N-CT in NMA	1.4512	374.0
CT-H1 in NMA	1.0949	370.0
C-CT in NMA	1.5227	345.0
CT-HC in NMA	1.0946	370.0
Parameters for angle bending		
angle[b]	θ_{eq} (Å)	Angle force constant (K_a, kcal·mol^{-1}·rad^{-2})
∠H-O-H in water	104.52	51.0
∠C-O-H in methanol	108.04	64.0
∠H-C-O in methanol	110.11	65.0
∠H-C-H in methanol	108.80	41.0
∠H-N-H in methylamine	106.31	40.5
∠C-N-H in methylamine	110.31	40.0
∠H-C-N in methylamine	111.80	66.0
∠H-C-H in methylamine	107.89	34.0
∠CT-C-O in NMA	121.71	80.00
∠CT-C-N in NMA	115.22	70.00
∠O-C-N in NMA	123.07	76.98
∠C-N-H in NMA	118.76	50.00
∠C-N-CT in NMA	122.59	50.00
∠H-N-CT in NMA	118.66	32.01
∠HC-CT-HC in NMA	108.36	39.57
∠HC-CT-C in NMA	110.52	45.85
∠N-CT-H1 in NMA	109.93	60.00
∠H1-CT-H1 in NMA	109.00	39.57

Parameters for bond angle coupling	strbnd force constant (K_{ba}, kcal·mol^{-1}· Å^{-1}· rad^{-1})	strbnd force constant (K_{ba}, kcal·mol^{-1}· Å^{-1}· rad^{-1})
H-O-H in water	35.60	35.60
C-O-H in methanol	38.00	-4.50
H-C-N in methylamine	12.50	12.50
C-N-H in methylamine	4.30	4.30
C-CT-HC in NMA	11.50	11.50
N-CT-H1 in NMA	11.50	11.50
CT-C-O in NMA	18.70	18.70
CT-C-N in NMA	18.70	18.70
O-C-N in NMA	18.70	18.70
CT-N-C in NMA	7.20	7.20
CT-N-H in NMA	4.30	4.30
C-N-H in NMA	4.30	4.30

Parameters for torsion

torsion	V_1			V_2			V_3		
	K_ϕ	n	γ	K_ϕ	n	γ	K_ϕ	n	γ
H-O-C-H in methanol	0.00	1	0	0.00	2	180	0.20	3	0
H-N-C-H in methylamine	0.00	1	0	0.44	2	180	0.25	3	0
HC-CT-C-N in NMA	0.00	1	0	0.00	2	180	0.00	3	0
HC-CT-C-O in NMA	0.00	1	0	0.00	2	180	0.00	3	0
CT-C-N-H in NMA	0.00	1	0	1.20	2	180	0.00	3	0
CT-C-N-CT in NMA	0.00	1	0	2.50	2	180	0.00	3	0
O-C-N-H in NMA	0.00	1	0	0.50	2	180	0.00	3	0
O-C-N-CT in NMA	0.00	1	0	0.50	2	180	0.00	3	0
C-N-CT-H1 in NMA	0.00	1	0	0.00	2	180	0.00	3	0
H-N-CT-H1 in NMA	0.00	1	0	0.00	2	180	0.00	3	0

Parameters for bond dipole moments and lone pairs		Dipole moment (debye)
μ_0(O-H)	O-H in water	1.51
μ_0(O-H)	O-H connected with the electron withdrawing group	1.78
μ_0(C-O)	C(sp^3)-O(sp^3)	0.70
μ_0(C-H)	C(sp^3)-H with electronegative neighbor N(sp^3) or O(sp^3)	0.70
μ_0(C-N)	C(sp^3)-N(sp^3)	0.70
μ_0(N-H)	N(sp^3)-H connected with the electron withdrawing group	1.51
μ_0(C=O)	double bond of C=O	2.65
μ_0(N-H)	N(sp^2)-H in conjugated system	1.51
μ_0(C-H)	C(sp^3)-H with no electronegative neighbor	1.25

μ_0(C-N)	single bond for C(sp^2)-N(sp^2)	0.45
μ_0(C-N)	single bond for C(sp^3)-N(sp^2)	1.20

Parameters for van der Waals interaction terms[c]	R^*(Å)	ε(kcal·mol^{-1})
O in water	1.6800	0. 1521
H in water	0.4500	0.0460
C in alcohol	1.9080	0.1094
H attached to a carbon in alcohol	1.0000	0.0157
O in alcohol	1.6690	0.1620
H attached to an oxygen in alcohol	0.6350	0.0157
C in methylamine	1.9080	0.1094
H attached to a carbon in methylamine	1.0000	0.0157
N in methylamine	1.6860	0.1700
H attached to a nitrogen in methylamine	1.0870	0.0157
sp^2 oxygen in carbonyl group	1.6612	0.2100
sp^2 carbon in carbonyl group	1.9080	0.0860
sp^2 nitrogen with no lone pair	1.7150	0.1700
H attached to sp^2 nitrogen	0.8450	0.0157
sp^3 carbon attach to carbonyl group	1.9080	0.1094
H attached to an sp^3 carbon with no electronegative neighbor	1.4000	0.0157
sp^3 carbon with an electronegative neighbor	1.9080	0.1094
H attached to an sp^3 carbon with electronegative neighbor	0.9500	0.0157

Parameters for orbital overlap term	D_m[d]	a_m[e]	$R_{eq,m}$[f]	p_m[g]	q_m[h]	α_m[i]
O-H···O(sp^2)	1.25	1.30	1.85	0.001	0.28	0.001
N-H···O(sp^2)	1.05	1.30	1.85	0.001	0.28	0.001
O-H···O(sp^3)	1.05	1.30	1.90	0.001	0.28	0.001
N-H···O(sp^3)	1.05	1.30	1.90	0.001	0.28	0.001
O-H···N(sp^3)	1.05	1.30	1.95	0.001	0.28	0.001
N-H··· N(sp^3)	1.05	1.30	1.95	0.001	0.28	0.001

[a] $K_{b1} = 2.55$, $K_{b2} = (7/12)\cdot K_{b1}^2$

[b] $K_{a1} = 0.006$, $K_{a2} = (7/12)\cdot K_{a1}^2$

[c] $A_{ij} = \varepsilon_{ij}\cdot(R_{ij}^*)^{12}$, $B_{ij} = 2\varepsilon_{ij}\cdot(R_{ij}^*)^6$, $R_{ij}^* = R_i^* + R_j^*$, $\varepsilon_{ij} = (\varepsilon_i\cdot\varepsilon_j)^{0.5}$

[d] D_m is the depth of the potential, in kcal·mol^{-1}

[e] a_m is the width of the potential

[f] $R_{eq,\,m}$ denotes the equilibrium hydrogen bond distance, in angstrom

[g] p_m is the minimum overlap integral

[h] q_m is the maximum overlap integral

[i] α_m is dependent on the type of hydrogen bond

Table S2 Interaction energies(kcal·mol^{-1}) of the HD16_2D data set obtained via various methods

water-water

	CCSD(T)/CBS	AMOEBA09	PBFF
01_water-water_090_-40 °	-2.05	-2.36	-3.80
01_water-water_090_-20 °	-4.03	-4.31	-5.16
01_water-water_090_-10 °	-4.44	-4.74	-5.39
01_water-water_090_0 °	-4.57	-4.89	-5.49
01_water-water_095_-40 °	-3.02	-3.30	-4.27
01_water-water_095_-20 °	-4.48	-4.74	-5.13
01_water-water_095_-10 °	-4.79	-5.06	-5.28
01_water-water_095_0 °	-4.88	-5.16	-5.35
01_water-water_100_-40 °	-3.49	-3.70	-4.31
01_water-water_100_-20 °	-4.60	-4.77	-4.87
01_water-water_100_-10 °	-4.83	-5.01	-4.97
01_water-water_100_0 °	-4.89	-5.08	-5.03
01_water-water_105_-40 °	-3.65	-3.77	-4.13
01_water-water_105_-20 °	-4.50	-4.59	-4.52
01_water-water_105_-10 °	-4.67	-4.77	-4.59
01_water-water_105_0 °	-4.72	-4.82	-4.64
01_water-water_110_-40 °	-3.61	-3.65	-3.85
01_water-water_110_-20 °	-4.27	-4.29	-4.14
01_water-water_110_-10 °	-4.41	-4.43	-4.19
01_water-water_110_0 °	-4.45	-4.47	-4.24
01_water-water_125_-40 °	-2.99	-2.88	-2.91
01_water-water_125_-20 °	-3.35	-3.23	-3.07
01_water-water_125_-10 °	-3.43	-3.31	-3.11
01_water-water_125_0 °	-3.46	-3.34	-3.15
01_water-water_150_-40 °	-1.83	-1.71	-1.72
01_water-water_150_-20 °	-2.03	-1.91	-1.84
01_water-water_150_-10 °	-2.08	-1.96	-1.88
01_water-water_150_0 °	-2.11	-1.98	-1.92
01_water-water_200_-40 °	-0.71	-0.67	-0.54
01_water-water_200_-20 °	-0.82	-0.78	-0.62
01_water-water_200_-10 °	-0.85	-0.81	-0.65
01_water-water_200_0 °	-0.87	-0.83	-0.68

water-methanol

	CCSD(T)/CBS	AMOEBA09	PBFF
02_water-methanol_090_-30 °	-3.42	-2.46	-2.92
02_water-methanol_090_-10 °	-5.03	-4.73	-4.99
02_water-methanol_090_0 °	-5.19	-5.10	-5.37
02_water-methanol_090_+10 °	-5.04	-5.09	-5.56
02_water-methanol_095_-30 °	-4.34	-3.77	-3.85
02_water-methanol_095_-10 °	-5.46	-5.38	-5.20
02_water-methanol_095_0 °	-5.55	-5.63	-5.45
02_water-methanol_095_+10 °	-5.41	-5.60	-5.59
02_water-methanol_100_-30 °	-4.74	-4.38	-4.17
02_water-methanol_100_-10 °	-5.52	-5.52	-5.07
02_water-methanol_100_0 °	-5.57	-5.68	-5.25
02_water-methanol_100_+10 °	-5.44	-5.64	-5.35
02_water-methanol_105_-30 °	-4.81	-4.54	-4.15
02_water-methanol_105_-10 °	-5.36	-5.36	-4.78
02_water-methanol_105_0 °	-5.38	-5.48	-4.91
02_water-methanol_105_+10 °	-5.27	-5.43	-5.00
02_water-methanol_110_-30 °	-4.68	-4.45	-3.97
02_water-methanol_110_-10 °	-5.07	-5.05	-4.42
02_water-methanol_110_0 °	-5.08	-5.13	-4.53
02_water-methanol_110_+10 °	-4.98	-5.08	-4.61
02_water-methanol_125_-30 °	-3.79	-3.59	-3.12
02_water-methanol_125_-10 °	-3.95	-3.86	-3.35
02_water-methanol_125_0 °	-3.94	-3.90	-3.42
02_water-methanol_125_+10 °	-3.89	-3.87	-3.47
02_water-methanol_150_-30 °	-2.30	-2.15	-1.88
02_water-methanol_150_-10 °	-2.38	-2.29	-2.03
02_water-methanol_150_0 °	-2.39	-2.32	-2.08
02_water-methanol_150_+10 °	-2.37	-2.31	-2.13
02_water-methanol_200_-30 °	-0.87	-0.83	-0.69
02_water-methanol_200_-10 °	-0.94	-0.92	-0.79
02_water-methanol_200_0 °	-0.95	-0.94	-0.82
02_water-methanol_200_+10 °	-0.96	-0.95	-0.85

water-methylamine

	CCSD(T)/CBS	AMOEBA09	PBFF
03_water-methylamine_090_-40 °	-3.04	-3.63	-5.00
03_water-methylamine_090_-20 °	-5.75	-7.12	-6.58
03_water-methylamine_090_-10 °	-6.33	-7.99	-6.88
03_water-methylamine_090_0 °	-6.49	-8.36	-7.03
03_water-methylamine_095_-40 °	-4.15	-4.90	-5.37
03_water-methylamine_095_-20 °	-6.27	-7.58	-6.41
03_water-methylamine_095_-10 °	-6.74	-8.27	-6.62
03_water-methylamine_095_0 °	-6.87	-8.56	-6.74
03_water-methylamine_100_-40 °	-4.70	-5.37	-5.29
03_water-methylamine_100_-20 °	-6.39	-7.47	-6.00
03_water-methylamine_100_-10 °	-6.76	-8.01	-6.16
03_water-methylamine_100_0 °	-6.88	-8.25	-6.26
03_water-methylamine_105_-40 °	-4.88	-5.38	-4.98
03_water-methylamine_105_-20 °	-6.24	-7.04	-5.51
03_water-methylamine_105_-10 °	-6.55	-7.48	-5.63
03_water-methylamine_105_0 °	-7.35	-7.68	-5.73
03_water-methylamine_110_-40 °	-4.82	-5.14	-4.59
03_water-methylamine_110_-20 °	-5.93	-6.48	-5.00
03_water-methylamine_110_-10 °	-6.19	-6.84	-5.11
03_water-methylamine_110_0 °	-6.28	-7.02	-5.19
03_water-methylamine_125_-40 °	-3.99	-3.91	-3.36
03_water-methylamine_125_-20 °	-4.67	-4.71	-3.63
03_water-methylamine_125_-10 °	-4.84	-4.94	-3.72
03_water-methylamine_125_0 °	-4.92	-5.07	-3.79
03_water-methylamine_150_-40 °	-2.40	-2.17	-1.90
03_water-methylamine_150_-20 °	-2.80	-2.63	-2.11
03_water-methylamine_150_-10 °	-2.91	-2.77	-2.19
03_water-methylamine_150_0 °	-2.98	-2.86	-2.25
03_water-methylamine_200_-40 °	-0.82	-0.70	-0.52
03_water-methylamine_200_-20 °	-1.02	-0.94	-0.66
03_water-methylamine_200_-10 °	-1.09	-1.02	-0.72
03_water-methylamine_200_0 °	-1.14	-1.08	-0.76

water-NMA

	CCSD(T)/CBS	AMOEBA09	PBFF
04_water-NMA_090_-30 °	-2.56	-0.66	-0.53
04_water-NMA_090_-10 °	-7.22	-6.67	-7.28
04_water-NMA_090_0 °	-7.63	-7.56	-7.85
04_water-NMA_090_+10 °	-7.47	-7.75	-7.88
04_water-NMA_095_-30 °	-4.66	-3.13	-3.71
04_water-NMA_095_-10 °	-7.82	-7.48	-7.96
04_water-NMA_095_0 °	-8.06	-8.08	-8.21
04_water-NMA_095_+10 °	-7.86	-8.14	-8.13
04_water-NMA_100_-30 °	-5.72	-4.57	-5.42
04_water-NMA_100_-10 °	-7.97	-7.68	-8.01
04_water-NMA_100_0 °	-8.08	-8.05	-8.07
04_water-NMA_100_+10 °	-7.86	-8.05	-7.92
04_water-NMA_105_-30 °	-6.26	-5.31	-6.26
04_water-NMA_105_-10 °	-7.82	-7.50	-7.75
04_water-NMA_105_0 °	-7.85	-7.73	-7.69
04_water-NMA_105_+10 °	-7.63	-7.68	-7.50
04_water-NMA_110_-30 °	-6.45	-5.61	-6.55
04_water-NMA_110_-10 °	-7.50	-7.13	-7.33
04_water-NMA_110_0 °	-7.46	-7.25	-7.19
04_water-NMA_110_+10 °	-7.25	-7.17	-6.99
04_water-NMA_125_-30 °	-5.87	-5.16	-5.98
04_water-NMA_125_-10 °	-6.11	-5.60	-5.82
04_water-NMA_125_0 °	-6.00	-5.58	-5.61
04_water-NMA_125_+10 °	-5.82	-5.48	-5.42
04_water-NMA_150_-30 °	-4.01	-3.40	-4.08
04_water-NMA_150_-10 °	-3.92	-3.44	-3.72
04_water-NMA_150_0 °	-3.83	-3.40	-3.56
04_water-NMA_150_+10 °	-3.72	-3.34	-3.42
04_water-NMA_200_-30 °	-1.68	-1.35	-1.74
04_water-NMA_200_-10 °	-1.66	-1.40	-1.58
04_water-NMA_200_0 °	-1.63	-1.41	-1.51
04_water-NMA_200_+10 °	-1.60	-1.40	-1.45

methanol-methanol

	CCSD(T)/CBS	AMOEBA09	PBFF
05_methanol-methanol_090_-40 °	-0.51	2.53	-0.42
05_methanol-methanol_090_-20 °	-4.49	-3.10	-5.11
05_methanol-methanol_090_-10 °	-5.08	-4.06	-5.67
05_methanol-methanol_090_0 °	-5.27	-4.48	-5.92
05_methanol-methanol_095_-40 °	-2.66	-0.95	-3.27
05_methanol-methanol_095_-20 °	-5.16	-4.35	-5.73
05_methanol-methanol_095_-10 °	-5.57	-5.00	-6.06
05_methanol-methanol_095_0 °	-5.69	-5.29	-6.21
05_methanol-methanol_100_-40 °	-3.73	-2.73	-4.38
05_methanol-methanol_100_-20 °	-5.37	-4.87	-5.75
05_methanol-methanol_100_-10 °	-5.66	-5.32	-5.95
05_methanol-methanol_100_0 °	-5.75	-5.52	-6.05
05_methanol-methanol_105_-40 °	-4.17	-3.55	-4.68
05_methanol-methanol_105_-20 °	-5.30	-4.95	-5.50
05_methanol-methanol_105_-10 °	-5.52	-5.28	-5.63
05_methanol-methanol_105_0 °	-5.58	-5.42	-5.69
05_methanol-methanol_110_-40 °	-4.26	-3.83	-4.59
05_methanol-methanol_110_-20 °	-5.07	-4.79	-5.12
05_methanol-methanol_110_-10 °	-5.23	-5.03	-5.21
05_methanol-methanol_110_0 °	-5.28	-5.14	-5.26
05_methanol-methanol_125_-40 °	-3.61	-3.38	-3.66
05_methanol-methanol_125_-20 °	-4.01	-3.79	-3.88
05_methanol-methanol_125_-10 °	-4.10	-3.92	-3.94
05_methanol-methanol_125_0 °	-4.13	-3.98	-3.97
05_methanol-methanol_-20 °_-40 °	-2.20	-2.06	-2.19
05_methanol-methanol_-20 °_-20 °	-2.43	-2.29	-2.34
05_methanol-methanol_-20 °_-10 °	-2.49	-2.36	-2.39
05_methanol-methanol_-20 °_0 °	-2.52	-2.40	-2.42
05_methanol-methanol_200_-40 °	-0.82	-0.79	-0.80
05_methanol-methanol_200_-20 °	-0.95	-0.92	-0.91
05_methanol-methanol_200_-10 °	-0.99	-0.97	-0.95
05_methanol-methanol_200_0 °	-1.01	-0.99	-0.97

methanol_methylamine

	CCSD(T)/CBS	AMOEBA09	PBFF
06_methanol_methylamine_090_-40 °	-3.97	-3.20	-7.19
06_methanol_methylamine_090_-20 °	-6.31	-6.21	-7.98
06_methanol_methylamine_090_-10 °	-6.85	-6.97	-8.03
06_methanol_methylamine_090_0 °	-6.97	-7.15	-7.89
06_methanol_methylamine_095_-40 °	-4.95	-4.66	-7.42
06_methanol_methylamine_095_-20 °	-6.85	-7.04	-7.92
06_methanol_methylamine_095_-10 °	-7.31	-7.68	-7.95
06_methanol_methylamine_095_0 °	-7.47	-7.89	-7.87
06_methanol_methylamine_100_-40 °	-5.40	-5.27	-7.15
06_methanol_methylamine_100_-20 °	-6.96	-7.18	-7.49
06_methanol_methylamine_100_-10 °	-7.36	-7.72	-7.51
06_methanol_methylamine_100_0 °	-7.54	-7.95	-7.46
06_methanol_methylamine_105_-40 °	-5.51	-5.37	-6.67
06_methanol_methylamine_105_-20 °	-6.79	-6.93	-6.91
06_methanol_methylamine_105_-10 °	-7.15	-7.39	-6.93
06_methanol_methylamine_105_0 °	-7.34	-7.63	-6.91
06_methanol_methylamine_110_-40 °	-5.39	-5.18	-6.11
06_methanol_methylamine_110_-20 °	-6.47	-6.47	-6.29
06_methanol_methylamine_110_-10 °	-6.78	-6.87	-6.31
06_methanol_methylamine_110_0 °	-6.97	-7.11	-6.31
06_methanol_methylamine_125_-40 °	-4.42	-4.03	-4.49
06_methanol_methylamine_125_-20 °	-5.12	-4.84	-4.61
06_methanol_methylamine_125_-10 °	-5.34	-5.11	-4.64
06_methanol_methylamine_125_0 °	-5.50	-5.31	-4.66
06_methanol_methylamine_150_-40 °	-2.68	-2.28	-2.61
06_methanol_methylamine_150_-20 °	-3.09	-2.75	-2.72
06_methanol_methylamine_150_-10 °	-3.23	-2.92	-2.75
06_methanol_methylamine_150_0 °	-3.35	-3.05	-2.78
06_methanol_methylamine_200_-40 °	-0.94	-0.76	-0.95
06_methanol_methylamine_200_-20 °	-1.14	-1.00	-1.04
06_methanol_methylamine_200_-10 °	-1.22	-1.08	-1.06
06_methanol_methylamine_200_0 °	-1.27	-1.15	-1.09

methanol-NMA

	CCSD(T)/CBS	AMOEBA09	PBFF
07_methanol-NMA_090_-30 °	-2.65	-1.33	-0.93
07_methanol-NMA_090_-10 °	-7.12	-6.59	-7.40
07_methanol-NMA_090_0 °	-7.62	-7.28	-7.59
07_methanol-NMA_090_+10 °	-7.50	-7.30	-7.24
07_methanol-NMA_095_-30 °	-4.58	-3.90	-4.40
07_methanol-NMA_095_-10 °	-7.84	-7.57	-8.42
07_methanol-NMA_095_0 °	-8.14	-7.97	-8.35
07_methanol-NMA_095_+10 °	-7.95	-7.88	-7.94
07_methanol-NMA_100_-30 °	-5.75	-5.39	-6.26
07_methanol-NMA_100_-10 °	-8.08	-7.87	-8.59
07_methanol-NMA_100_0 °	-8.22	-8.07	-8.36
07_methanol-NMA_100_+10 °	-7.99	-7.91	-7.92
07_methanol-NMA_105_-30 °	-6.38	-6.15	-7.15
07_methanol-NMA_105_-10 °	-8.00	-7.76	-8.34
07_methanol-NMA_105_0 °	-8.03	-7.82	-8.02
07_methanol-NMA_105_+10 °	-7.77	-7.62	-7.57
07_methanol-NMA_110_-30 °	-6.64	-6.44	-7.45
07_methanol-NMA_110_-10 °	-7.72	-7.42	-7.88
07_methanol-NMA_110_0 °	-7.67	-7.15	-7.07
07_methanol-NMA_110_+10 °	-7.40	-7.15	-7.07
07_methanol-NMA_125_-30 °	-6.19	-5.89	-6.74
07_methanol-NMA_125_-10 °	-6.36	-5.89	-6.21
07_methanol-NMA_125_0 °	-6.19	-5.73	-5.82
07_methanol-NMA_125_+10 °	-5.93	-5.50	-5.44
07_methanol-NMA_150_-30 °	-4.33	-3.89	-4.52
07_methanol-NMA_150_-10 °	-4.12	-3.62	-3.89
07_methanol-NMA_150_0 °	-3.95	-3.48	-3.60
07_methanol-NMA_150_+10 °	-3.75	-3.32	-3.34
07_methanol-NMA_200_-30 °	-1.83	-1.54	-1.86
07_methanol-NMA_200_-10 °	-1.71	-1.46	-1.57
07_methanol-NMA_200_0 °	-1.63	-1.41	-1.44
07_methanol-NMA_200_+10 °	-1.54	-1.35	-1.31

methanol-water

	CCSD(T)/CBS	AMOEBA09	PBFF
08_methanol-water_090_-40 °	-2.21	-1.82	-4.99
08_methanol-water_090_-20 °	-4.07	-3.66	-5.84
08_methanol-water_090_-10 °	-4.47	-4.09	-5.91
08_methanol-water_090_0 °	-4.59	-4.24	-5.84
08_methanol-water_095_-40 °	-3.12	-2.88	-5.41
08_methanol-water_095_-20 °	-4.54	-4.28	-5.91
08_methanol-water_095_-10 °	-4.85	-4.61	-5.93
08_methanol-water_095_0 °	-4.95	-4.73	-5.87
08_methanol-water_100_-40 °	-3.56	-3.36	-5.35
08_methanol-water_100_-20 °	-4.67	-4.44	-5.65
08_methanol-water_100_-10 °	-4.91	-4.71	-5.65
08_methanol-water_100_0 °	-5.00	-4.81	-5.60
08_methanol-water_105_-40 °	-3.70	-3.51	-5.07
08_methanol-water_105_-20 °	-4.58	-4.35	-5.26
08_methanol-water_105_-10 °	-4.78	-4.57	-5.25
08_methanol-water_105_0 °	-4.85	-4.65	-5.20
08_methanol-water_110_-40 °	-3.66	-3.44	-4.70
08_methanol-water_110_-20 °	-4.36	-4.13	-4.82
08_methanol-water_110_-10 °	-4.52	-4.30	-4.81
08_methanol-water_110_0 °	-4.59	-4.37	-4.77
08_methanol-water_125_-40 °	-3.03	-2.79	-3.53
08_methanol-water_125_-20 °	-3.44	-3.19	-3.59
08_methanol-water_125_-10 °	-3.54	-3.30	-3.58
08_methanol-water_125_0 °	-3.59	-3.35	-3.56
08_methanol-water_150_-40 °	-1.87	-1.68	-2.11
08_methanol-water_150_-20 °	-2.11	-1.92	-2.16
08_methanol-water_150_-10 °	-2.17	-1.99	-2.16
08_methanol-water_150_0 °	-2.20	-2.02	-2.16
08_methanol-water_200_-40 °	-0.73	-0.67	-0.79
08_methanol-water_200_-20 °	-0.85	-0.79	-0.84
08_methanol-water_200_-10 °	-0.89	-0.83	-0.85
08_methanol-water_200_0 °	-0.91	-0.85	-0.86

methylamine-methanol

	CCSD(T)/CBS	AMOEBA09	PBFF
09_methylamine-methanol_090_-40 °	-1.98	-1.82	-2.84
09_methylamine-methanol_090_-20 °	-2.60	-2.31	-2.86
09_methylamine-methanol_090_-10 °	-2.78	-2.47	-2.84
09_methylamine-methanol_090_0 °	-2.81	-2.53	-2.76
09_methylamine-methanol_095_-40 °	-2.31	-2.22	-3.23
09_methylamine-methanol_095_-20 °	-2.79	-2.60	-3.22
09_methylamine-methanol_095_-10 °	-2.96	-2.76	-3.21
09_methylamine-methanol_095_0 °	-3.04	-2.86	-3.17
09_methylamine-methanol_100_-40 °	-2.40	-2.32	-3.20
09_methylamine-methanol_100_-20 °	-2.78	-2.62	-3.18
09_methylamine-methanol_100_-10 °	-2.93	-2.77	-3.17
09_methylamine-methanol_100_0 °	-3.04	-2.89	-3.15
09_methylamine-methanol_105_-40 °	-2.35	-2.25	-3.01
09_methylamine-methanol_105_-20 °	-2.65	-2.50	-2.98
09_methylamine-methanol_105_-10 °	-2.78	-2.63	-2.97
09_methylamine-methanol_105_0 °	-2.90	-2.76	-2.96
09_methylamine-methanol_110_-40 °	-2.22	-2.10	-2.75
09_methylamine-methanol_110_-20 °	-2.46	-2.30	-2.71
09_methylamine-methanol_110_-10 °	-2.58	-2.42	-2.71
09_methylamine-methanol_110_0 °	-2.69	-2.54	-2.70
09_methylamine-methanol_125_-40 °	-1.68	-1.54	-1.98
09_methylamine-methanol_125_-20 °	-1.82	-1.66	-1.94
09_methylamine-methanol_125_-10 °	-1.89	-1.73	-1.93
09_methylamine-methanol_125_0 °	-1.98	-1.82	-1.93
09_methylamine-methanol_150_-40 °	-0.96	-0.86	-1.10
09_methylamine-methanol_150_-20 °	-1.02	-0.91	-1.08
09_methylamine-methanol_150_-10 °	-1.06	-0.95	-1.07
09_methylamine-methanol_150_0 °	-1.10	-1.00	-1.06
09_methylamine-methanol_200_-40 °	-0.36	-0.32	-0.34
09_methylamine-methanol_200_-20 °	-0.37	-0.34	-0.33
09_methylamine-methanol_200_-10 °	-0.38	-0.35	-0.32
09_methylamine-methanol_200_0 °	-0.39	-0.36	-0.31

methylamine-methylamine

	CCSD(T)/CBS	AMOEBA09	PBFF
10_methylamine-methylamine_090_-40 °	-2.31	-1.26	-3.74
10_methylamine-methylamine_090_-20 °	-3.47	-1.79	-3.87
10_methylamine-methylamine_090_-10 °	-3.75	-1.77	-3.87
10_methylamine-methylamine_090_0 °	-3.70	-1.37	-3.75
10_methylamine-methylamine_095_-40 °	-2.78	-2.17	-4.06
10_methylamine-methylamine_095_-20 °	-3.75	-2.66	-4.17
10_methylamine-methylamine_095_-10 °	-4.03	-2.73	-4.20
10_methylamine-methylamine_095_0 °	-4.09	-2.58	-4.16
10_methylamine-methylamine_100_-40 °	-2.96	-2.59	-3.94
10_methylamine-methylamine_100_-20 °	-3.76	-3.02	-4.04
10_methylamine-methylamine_100_-10 °	-4.02	-3.14	-4.07
10_methylamine-methylamine_100_0 °	-4.15	-3.13	-4.07
10_methylamine-methylamine_105_-40 °	-2.95	-2.70	-3.65
10_methylamine-methylamine_105_-20 °	-3.61	-3.08	-3.73
10_methylamine-methylamine_105_-10 °	-3.85	-3.22	-3.76
10_methylamine-methylamine_105_0 °	-4.01	-3.29	-3.78
10_methylamine-methylamine_110_-40 °	-2.83	-2.63	-3.31
10_methylamine-methylamine_110_-20 °	-3.37	-2.97	-3.36
10_methylamine-methylamine_110_-10 °	-3.59	-3.11	-3.39
10_methylamine-methylamine_110_0 °	-3.75	-3.22	-3.42
10_methylamine-methylamine_125_-40 °	-2.21	-2.07	-2.33
10_methylamine-methylamine_125_-20 °	-2.52	-2.28	-2.35
10_methylamine-methylamine_125_-10 °	-2.66	-2.38	-2.36
10_methylamine-methylamine_125_0 °	-2.79	-2.49	-2.37
10_methylamine-methylamine_150_-40 °	-1.30	-1.19	-1.27
10_methylamine-methylamine_150_-20 °	-1.42	-1.28	-1.26
10_methylamine-methylamine_150_-10 °	-1.48	-1.32	-1.26
10_methylamine-methylamine_150_0 °	-1.54	-1.37	-1.24
10_methylamine-methylamine_200_-40 °	-0.48	-0.44	-0.39
10_methylamine-methylamine_200_-20 °	-0.50	-0.45	-0.36
10_methylamine-methylamine_200_-10 °	-0.51	-0.46	-0.35
10_methylamine-methylamine_200_0 °	-0.51	-0.45	-0.33

methylamine-NMA

	CCSD(T)/CBS	AMOEBA09	PBFF
11_methylamine-NMA_090_-10 °	-3.88	-1.67	-3.77
11_methylamine-NMA_090_0 °	-4.95	-3.69	-4.94
11_methylamine-NMA_090_+10 °	-5.12	-4.19	-5.17
11_methylamine-NMA_090_+20 °	-4.94	-4.13	-5.05
11_methylamine-NMA_090_+30 °	-4.60	-3.86	-4.82
11_methylamine-NMA_095_-10 °	-4.80	-3.32	-5.20
11_methylamine-NMA_095_0 °	-5.36	-4.50	-5.73
11_methylamine-NMA_095_+10 °	-5.30	-4.63	-5.70
11_methylamine-NMA_095_+20 °	-5.03	-4.42	-5.48
11_methylamine-NMA_095_+30 °	-4.67	-4.11	-5.22
11_methylamine-NMA_100_-10 °	-5.21	-4.18	-5.68
11_methylamine-NMA_100_0 °	-5.41	-4.77	-5.82
11_methylamine-NMA_100_+10 °	-5.20	-4.67	-5.64
11_methylamine-NMA_100_+20 °	-4.89	-4.39	-5.37
11_methylamine-NMA_100_+30 °	-4.54	-4.05	-5.11
11_methylamine-NMA_105_-10 °	-5.28	-4.52	-5.68
11_methylamine-NMA_105_0 °	-5.24	-4.72	-5.58
11_methylamine-NMA_105_+10 °	-4.95	-4.49	-5.32
11_methylamine-NMA_105_+20 °	-4.61	-4.16	-5.03
11_methylamine-NMA_105_+30 °	-4.28	-3.83	-4.77
11_methylamine-NMA_110_-10 °	-5.14	-4.55	-5.44
11_methylamine-NMA_110_0 °	-4.94	-4.49	-5.20
11_methylamine-NMA_110_+10 °	-4.61	-4.19	-4.89
11_methylamine-NMA_110_+20 °	-4.28	-3.85	-4.61
11_methylamine-NMA_110_+30 °	-3.96	-3.54	-4.37
11_methylamine-NMA_125_-10 °	-4.17	-3.77	-4.25
11_methylamine-NMA_125_0 °	-3.80	-3.43	-3.89
11_methylamine-NMA_125_+10 °	-3.47	-3.10	-3.60
11_methylamine-NMA_125_+20 °	-3.20	-2.81	-3.36
11_methylamine-NMA_125_+30 °	-2.96	-2.57	-3.18
11_methylamine-NMA_150_-10 °	-2.50	-2.21	-2.53
11_methylamine-NMA_150_0 °	-2.22	-1.93	-2.27
11_methylamine-NMA_150_+10 °	-2.01	-1.72	-2.08
11_methylamine-NMA_150_+20 °	-1.85	-1.56	-1.94
11_methylamine-NMA_150_+30 °	-1.72	-1.43	-1.84
11_methylamine-NMA_200_-10 °	-0.88	-0.73	-0.88
11_methylamine-NMA_200_0 °	-0.80	-0.65	-0.79
11_methylamine-NMA_200_+10 °	-0.74	-0.60	-0.73
11_methylamine-NMA_200_+20 °	-0.69	-0.55	-0.68
11_methylamine-NMA_200_+30 °	-0.65	-0.52	-0.65

methylamine-water

	CCSD(T)/CBS	AMOEBA09	PBFF
12_methylamine-water_090_-30 °	-3.77	-1.03	-2.48
12_methylamine-water_090_-10 °	-6.48	-5.29	-6.27
12_methylamine-water_090_0 °	-6.75	-5.97	-6.92
12_methylamine-water_090_+10 °	-6.55	-6.02	-7.25
12_methylamine-water_095_-30 °	-5.13	-3.46	-3.97
12_methylamine-water_095_-10 °	-7.04	-6.47	-6.42
12_methylamine-water_095_0 °	-7.20	-6.92	-6.85
12_methylamine-water_095_+10 °	-7.02	-6.91	-7.09
12_methylamine-water_100_-30 °	-5.80	-4.75	-4.56
12_methylamine-water_100_-10 °	-7.15	-6.87	-6.18
12_methylamine-water_100_0 °	-7.25	-7.17	-6.48
12_methylamine-water_100_+10 °	-7.08	-7.13	-6.66
12_methylamine-water_105_-30 °	-6.01	-5.30	-4.65
12_methylamine-water_105_-10 °	-6.98	-6.80	-5.77
12_methylamine-water_105_0 °	-7.03	-7.01	-5.99
12_methylamine-water_105_+10 °	-6.88	-6.96	-6.13
12_methylamine-water_110_-30 °	-5.68	-5.41	-4.49
12_methylamine-water_110_-10 °	-6.41	-6.48	-5.29
12_methylamine-water_110_0 °	-6.45	-6.62	-5.47
12_methylamine-water_110_+10 °	-6.32	-6.57	-5.59
12_methylamine-water_125_-30 °	-4.77	-4.57	-3.51
12_methylamine-water_125_-10 °	-5.09	-5.02	-3.91
12_methylamine-water_125_0 °	-5.11	-5.08	-4.02
12_methylamine-water_125_+10 °	-5.04	-5.04	-4.11
12_methylamine-water_150_-30 °	-2.91	-2.72	-2.04
12_methylamine-water_150_-10 °	-3.08	-2.94	-2.29
12_methylamine-water_150_0 °	-3.11	-2.98	-2.37
12_methylamine-water_150_+10 °	-3.10	-2.98	-2.44
12_methylamine-water_200_-30 °	-1.02	-0.95	-0.68
12_methylamine-water_200_-10 °	-1.15	-1.09	-0.84
12_methylamine-water_200_0 °	-1.18	-1.13	-0.89
12_methylamine-water_200_+10 °	-1.20	-1.15	-0.94

NMA-methanol

	CCSD(T)/CBS	AMOEBA09	PBFF
13_NMA-methanol_090_-30 °	-3.34	-1.45	-4.04
13_NMA-methanol_090_-10 °	-5.41	-4.36	-5.54
13_NMA-methanol_090_0 °	-5.63	-4.80	-5.71
13_NMA-methanol_090_+10 °	-5.61	-4.85	-5.73
13_NMA-methanol_095_-30 °	-4.55	-3.63	-5.53
13_NMA-methanol_095_-10 °	-5.96	-5.54	-6.37
13_NMA-methanol_095_0 °	-6.11	-5.80	-6.43
13_NMA-methanol_095_+10 °	-6.02	-5.77	-6.41
13_NMA-methanol_100_-30 °	-5.17	-4.81	-6.04
13_NMA-methanol_100_-10 °	-6.11	-6.04	-6.48
13_NMA-methanol_100_0 °	-6.18	-6.17	-6.48
13_NMA-methanol_100_+10 °	-6.07	-6.10	-6.44
13_NMA-methanol_105_-30 °	-5.39	-5.34	-6.05
13_NMA-methanol_105_-10 °	-6.01	-6.11	-6.26
13_NMA-methanol_105_0 °	-6.03	-6.16	-6.23
13_NMA-methanol_105_+10 °	-5.91	-6.07	-6.17
13_NMA-methanol_110_-30 °	-5.36	-5.48	-5.81
13_NMA-methanol_110_-10 °	-5.75	-5.94	-5.89
13_NMA-methanol_110_0 °	-5.74	-5.94	-5.84
13_NMA-methanol_110_+10 °	-5.63	-5.83	-5.78
13_NMA-methanol_125_-30 °	-4.59	-4.78	-4.66
13_NMA-methanol_125_-10 °	-4.65	-4.84	-4.61
13_NMA-methanol_125_0 °	-4.61	-4.78	-4.56
13_NMA-methanol_125_+10 °	-4.50	-4.68	-4.50
13_NMA-methanol_150_-30 °	-3.00	-3.09	-2.97
13_NMA-methanol_150_-10 °	-2.99	-3.07	-2.94
13_NMA-methanol_150_0 °	-2.95	-3.03	-2.91
13_NMA-methanol_150_+10 °	-2.88	-2.96	-2.87
13_NMA-methanol_200_-30 °	-1.30	-1.33	-1.18
13_NMA-methanol_200_-10 °	-1.31	-1.35	-1.19
13_NMA-methanol_200_0 °	-1.20	-1.34	-1.19
13_NMA-methanol_200_+10 °	-1.28	-1.32	-1.18

NMA-methylamine

	CCSD(T)/CBS	AMOEBA09	PBFF
14_NMA-methylamine_090_-40 °	-1.87	0.75	-4.44
14_NMA-methylamine_090_-20 °	-5.75	-4.54	-7.03
14_NMA-methylamine_090_-10 °	-6.54	-5.57	-7.40
14_NMA-methylamine_090_0 °	-6.81	-5.97	-7.55
14_NMA-methylamine_095_-40 °	-3.75	-2.52	-5.94
14_NMA-methylamine_095_-20 °	-6.57	-6.15	-7.50
14_NMA-methylamine_095_-10 °	-7.15	-6.86	-7.72
14_NMA-methylamine_095_0 °	-7.34	-7.11	-7.81
14_NMA-methylamine_100_-40 °	-4.83	-4.36	-6.41
14_NMA-methylamine_100_-20 °	-6.89	-6.84	-7.35
14_NMA-methylamine_100_-10 °	-7.32	-7.32	-7.49
14_NMA-methylamine_100_0 °	-7.45	-7.49	-7.54
14_NMA-methylamine_105_-40 °	-5.38	-5.29	-6.36
14_NMA-methylamine_105_-20 °	-6.88	-6.97	-6.93
14_NMA-methylamine_105_-10 °	-7.20	-7.30	-7.02
14_NMA-methylamine_105_0 °	-7.29	-7.41	-7.06
14_NMA-methylamine_110_-40 °	-5.56	-5.64	-6.06
14_NMA-methylamine_110_-20 °	-6.66	-6.78	-6.41
14_NMA-methylamine_110_-10 °	-6.90	-7.01	-6.46
14_NMA-methylamine_110_0 °	-6.97	-7.08	-6.50
14_NMA-methylamine_125_-40 °	-5.02	-5.09	-4.73
14_NMA-methylamine_125_-20 °	-5.47	-5.46	-4.83
14_NMA-methylamine_125_-10 °	-5.58	-5.55	-4.86
14_NMA-methylamine_125_0 °	-5.61	-5.58	-4.89
14_NMA-methylamine_-20 °_-40 °	-3.34	-3.24	-2.90
14_NMA-methylamine_-20 °_-20 °	-3.49	-3.35	-2.95
14_NMA-methylamine_-20 °_-10 °	-3.53	-3.40	-2.99
14_NMA-methylamine_-20 °_0 °	-3.55	-3.42	-3.02
14_NMA-methylamine_200_-40 °	-1.39	-1.30	-1.07
14_NMA-methylamine_200_-20 °	-1.45	-1.38	-1.14
14_NMA-methylamine_200_-10 °	-1.48	-1.41	-1.17
14_NMA-methylamine_200_0 °	-1.49	-1.42	-1.19

NMA-NMA

	CCSD(T)/CBS	AMOEBA09	PBFF
15_NMA-NMA_090_-30 °	-4.37	-2.72	-5.19
15_NMA-NMA_090_-10 °	-7.61	-7.60	-7.31
15_NMA-NMA_090_0 °	-8.02	-8.19	-7.10
15_NMA-NMA_090_+10 °	-7.92	-8.21	-6.64
15_NMA-NMA_095_-30 °	-6.02	-5.24	-7.59
15_NMA-NMA_095_-10 °	-8.29	-8.56	-8.55
15_NMA-NMA_095_0 °	-8.53	-8.91	-8.24
15_NMA-NMA_095_+10 °	-8.40	-8.85	-7.80
15_NMA-NMA_100_-30 °	-6.95	-6.62	-8.53
15_NMA-NMA_100_-10 °	-8.50	-8.82	-8.76
15_NMA-NMA_100_0 °	-8.63	-9.01	-8.41
15_NMA-NMA_100_+10 °	-8.47	-8.91	-7.99
15_NMA-NMA_105_-30 °	-7.37	-7.26	-8.70
15_NMA-NMA_105_-10 °	-8.40	-8.66	-8.50
15_NMA-NMA_105_0 °	-8.45	-8.74	-8.14
15_NMA-NMA_105_+10 °	-8.29	-8.62	-7.74
15_NMA-NMA_110_-30 °	-7.46	-7.41	-8.48
15_NMA-NMA_110_-10 °	-8.11	-8.27	-8.02
15_NMA-NMA_110_0 °	-8.10	-8.28	-7.66
15_NMA-NMA_110_+10 °	-7.93	-8.14	-7.29
15_NMA-NMA_125_-30 °	-6.69	-6.54	-6.96
15_NMA-NMA_125_-10 °	-6.74	-6.61	-6.29
15_NMA-NMA_125_0 °	-6.66	-6.53	-5.99
15_NMA-NMA_125_+10 °	-6.51	-6.41	-5.70
15_NMA-NMA_150_-30 °	-4.65	-4.33	-4.51
15_NMA-NMA_150_-10 °	-4.50	-4.20	-3.99
15_NMA-NMA_150_0 °	-4.42	-4.13	-3.78
15_NMA-NMA_150_+10 °	-4.31	-4.05	-3.60
15_NMA-NMA_200_-30 °	-2.14	-1.89	-1.93
15_NMA-NMA_200_-10 °	-2.05	-1.85	-1.70
15_NMA-NMA_200_0 °	-2.01	-1.83	-1.60
15_NMA-NMA_200_+10 °	-1.95	-1.79	-1.50

NMA-water

	CCSD(T)/CBS	AMOEBA09	PBFF
16_NMA-water_090_-40 °	-2.67	-1.19	-3.81
16_NMA-water_090_-20 °	-4.19	-3.43	-5.21
16_NMA-water_090_-10 °	-4.56	-4.00	-5.52
16_NMA-water_090_0 °	-4.69	-4.34	-5.72
16_NMA-water_095_-40 °	-3.60	-2.57	-4.60
16_NMA-water_095_-20 °	-4.67	-4.20	-5.55
16_NMA-water_095_-10 °	-4.93	-4.64	-5.79
16_NMA-water_095_0 °	-5.06	-4.94	-5.98
16_NMA-water_100_-40 °	-4.05	-3.29	-4.77
16_NMA-water_100_-20 °	-4.79	-4.48	-5.43
16_NMA-water_100_-10 °	-5.00	-4.83	-5.63
16_NMA-water_100_0 °	-5.12	-5.10	-5.82
16_NMA-water_105_-40 °	-4.19	-3.59	-4.65
16_NMA-water_105_-20 °	-4.71	-4.47	-5.12
16_NMA-water_105_-10 °	-4.87	-4.75	-5.29
16_NMA-water_105_0 °	-4.98	-5.00	-5.48
16_NMA-water_110_-40 °	-4.15	-3.64	-4.39
16_NMA-water_110_-20 °	-4.50	-4.29	-4.74
16_NMA-water_110_-10 °	-4.63	-4.53	-4.90
16_NMA-water_110_0 °	-4.75	-4.75	-5.08
16_NMA-water_125_-40 °	-3.51	-3.12	-3.42
16_NMA-water_125_-20 °	-3.62	-3.43	-3.61
16_NMA-water_125_-10 °	-3.69	-3.58	-3.73
16_NMA-water_125_0 °	-6.15	-3.75	-3.90
16_NMA-water_150_-40 °	-2.33	-2.05	-2.14
16_NMA-water_150_-20 °	-2.34	-2.18	-2.26
16_NMA-water_150_-10 °	-2.38	-2.27	-2.36
16_NMA-water_150_0 °	-2.45	-2.38	-2.49
16_NMA-water_200_-40 °	-1.08	-0.96	-0.83
16_NMA-water_200_-20 °	-1.09	-1.02	-0.92
16_NMA-water_200_-10 °	-1.11	-1.05	-0.98
16_NMA-water_200_0 °	-1.13	-1.09	-1.06

Table S3 Optimized monomer coordinates obtained using different methods

Method-01-MP2/aug-cc-pVTZ-Single-Water			
8	0.0000000	0.1182390	0.0000000
1	0.7581030	-0.4729560	0.0000000
1	-0.7581030	-0.4729570	0.0000000
Method-02-MP2/cc-pVTZ-Single-Water			
8	0.0000000	0.0000000	0.1187280
1	0.0000000	0.7533060	-0.4749100
1	0.0000000	-0.7533060	-0.4749100
Method-03-B3LYP/cc-pVTZ-Single-Water			
8	0.0000000	0.0000000	0.1176690
1	0.0000000	0.7602840	-0.4706760
1	0.0000000	-0.7602840	-0.4706760
Method-04-M06-2X/cc-pVTZ-Single-Water			
8	0.0000000	0.0000000	0.1168700
1	0.0000000	0.7605000	-0.4674790
1	0.0000000	-0.7605000	-0.4674790
Method-05-AMOEBA09-Single-Water			
8	0.0000000	0.0000000	0.1117310
1	0.0000000	-0.7775550	-0.4469250
1	0.0000000	0.7775550	-0.4469250
Method-06-PBFF-Single-Water			
8	0.0000000	0.1171760	0.0000000
1	0.7569470	-0.4687050	0.0000000
1	-0.7569470	-0.4687020	0.0000000

Method-01-MP2/aug-cc-pVTZ-Single-Methanol

8	0.7492440	0.1222120	0.0000100
1	1.1366160	-0.7573500	0.0000190
6	-0.6673070	-0.0200440	0.0000110
1	-1.0790940	0.9847880	-0.0027190
1	-1.0236150	-0.5447240	-0.8880400
1	-1.0240130	-0.5401480	0.8905940

Method-02-MP2/cc-pVTZ-Single-Methanol

8	0.7480610	0.1217700	0.0000100
1	1.1256390	-0.7602980	0.0000590
6	-0.6626680	-0.0195280	0.0000110
1	-1.0785640	0.9833130	-0.0033910
1	-1.0275160	-0.5428740	-0.8855300
1	-1.0280410	-0.5371340	0.8887180

Method-03-B3LYP/cc-pVTZ-Single-Methanol

8	0.7482540	0.1218410	0.0000100
1	1.1434030	-0.7538140	0.0000650
6	-0.6640360	-0.0200640	0.0000080
1	-1.0829510	0.9848580	-0.0034850
1	-1.0308640	-0.5456500	-0.8880720
1	-1.0314050	-0.5397380	0.8913640

Method-04-M06-2X/cc-pVTZ-Single-Methanol

8	0.7442370	0.1221000	0.0000150
1	1.1412450	-0.7501970	0.0000590
6	-0.6609550	-0.0202700	0.0000130
1	-1.0829130	0.9824820	-0.0039180
1	-1.0229130	-0.5470350	-0.8873100
1	-1.0235850	-0.5404290	0.8909760

Method-05-AMOEBA09-Single-Methanol

8	0.7435000	0.1295410	-0.0000010
1	1.1283360	-0.7581760	0.0000100
6	-0.6604180	-0.0187050	0.0000020
1	-1.1414510	0.9840370	-0.0000750
1	-0.9861760	-0.5750460	-0.9070310
1	-0.9861980	-0.5749150	0.9070940

Method-06-PBFF-Single-Methanol

8	0.7490720	0.1282510	-0.0000070
1	1.1375850	-0.7515430	0.0000630
6	-0.6685430	-0.0179880	-0.0000060
1	-1.1440500	0.9590020	-0.0008400
1	-0.9873350	-0.5635290	-0.8837000
1	-0.9875180	-0.5620060	0.8845660

Method-01-MP2/aug-cc-pVTZ-Single-Methylamine

7	-0.7492790	-0.0000370	-0.1230390
1	-1.1467100	-0.8098270	0.3355720
1	-1.1465040	0.8098380	0.3355980
6	0.7073230	-0.0000420	0.0178740
1	1.1114440	0.8794240	-0.4794860
1	1.0702960	-0.0044710	1.0498640
1	1.1124900	-0.8744500	-0.4875220

Method-02-MP2/cc-pVTZ-Single-Methylamine

7	-0.7504700	-0.0000200	-0.1263420
1	-1.1373440	-0.8059110	0.3467460
1	-1.1371770	0.8059210	0.3467970
6	0.7051570	-0.0000260	0.0180500
1	1.1123750	0.8765580	-0.4806580
1	1.0714970	-0.0026600	1.0486120
1	1.1129970	-0.8736140	-0.4854020

Method-03-B3LYP/cc-pVTZ-Single-Methylamine

7	-0.7504540	-0.0000380	-0.1224970
1	-1.1487010	-0.8107270	0.3352410
1	-1.1485150	0.8107110	0.3352940
6	0.7063540	-0.0000400	0.0176300
1	1.1158120	0.8794180	-0.4806190
1	1.0795680	-0.0044410	1.0503860
1	1.1168890	-0.8744550	-0.4886050

Method-04-M06-2X/cc-pVTZ-Single-Methylamine

7	-0.7484800	-0.0000480	-0.1231210
1	-1.1443720	-0.8098840	0.3361000
1	-1.1440750	0.8099500	0.3360460
6	0.7045920	-0.0000610	0.0176700
1	1.1133880	0.8796890	-0.4778480
1	1.0722060	-0.0058220	1.0498960
1	1.1146610	-0.8732290	-0.4883660

Method-05-AMOEBA09-Single-Methylamine

7	-0.7465170	-0.0000010	-0.1252510
1	-1.1565740	-0.8090030	0.3190020
1	-1.1565720	0.8090070	0.3189980
6	0.7130450	0.0000000	0.0145100
1	1.1340180	0.8834520	-0.4565180
1	0.9924590	0.0000030	1.0647240
1	1.1340170	-0.8834540	-0.4565140

Method-06-PBFF-Single-Methylamine

7	-0.7511420	0.0000010	-0.1271860
1	-1.1496050	-0.8122250	0.3271890
1	-1.1496270	0.8122110	0.3272010

6	0.7074100	0.0000020	0.0117950
1	1.1535570	0.8824930	-0.4481300
1	1.0056450	-0.0000700	1.0615180
1	1.1535650	-0.8824270	-0.4482430

Method-01-MP2/aug-cc-pVTZ-Single-NMA

6	1.8250150	-0.5268630	-0.0000240
1	1.7556930	-1.6127860	0.0000990
1	2.3778450	-0.2014920	0.8786970
1	2.3776180	-0.2016800	-0.8789590
6	0.4794890	0.1576480	0.0000400
8	0.3629110	1.3791740	0.0000100
7	-0.6055080	-0.6604430	0.0000040
1	-0.4736800	-1.6551810	0.0001890
6	-1.9442960	-0.1053670	-0.0000230
1	-2.1009880	0.5143720	0.8811290
1	-2.1006600	0.5151400	-0.8806930
1	-2.6618090	-0.9211760	-0.0005270

Method-02-MP2/cc-pVTZ-Single-NMA

6	-1.8058250	-0.5611080	0.0023500
1	-1.7090710	-1.6442440	-0.0078120
1	-2.3741550	-0.2441540	-0.8684460
1	-2.3623040	-0.2591820	0.8861250
6	-0.4807710	0.1652740	-0.0008110
8	-0.4137540	1.3869260	-0.0004750
7	0.6187230	-0.6389970	-0.0091420
1	0.4825240	-1.6323360	0.0170930
6	1.9613920	-0.1027800	0.0034400
1	1.8761590	0.9715080	-0.1258190
1	2.4649990	-0.3051800	0.9476640
1	2.5520480	-0.5171570	-0.8108790

Method-03-B3LYP/cc-pVTZ-Single-NMA

6	-1.8117930	-0.5656600	0.0000020
1	-1.7184620	-1.6514350	-0.0001280
1	-2.3782910	-0.2571710	-0.8778440
1	-2.3781480	-0.2573890	0.8780220
6	-0.4831590	0.1665240	-0.0000070
8	-0.4252010	1.3839230	-0.0000030
7	0.6233390	-0.6304140	0.0000010
1	0.4945890	-1.6262200	-0.0000460
6	1.9735220	-0.1019600	0.0000050
1	1.9001080	0.9820470	0.0000050
1	2.5235150	-0.4208710	0.8873360
1	2.5235020	-0.4208670	-0.8873340

Method-04-M06-2X/cc-pVTZ-Single-NMA

6	-1.8089920	-0.5575080	0.0020430
1	-1.7163040	-1.6415850	-0.0191770
1	-2.3791850	-0.2267590	-0.8637590
1	-2.3588670	-0.2592870	0.8926210

6	-0.4805620	0.1642640	-0.0009190
8	-0.4158550	1.3763050	-0.0003980
7	0.6197480	-0.6350020	-0.0079180
1	0.4887090	-1.6296780	0.0169420
6	1.9640320	-0.1000090	0.0029990
1	1.8881090	0.9715610	-0.1588980
1	2.4580510	-0.2771400	0.9591820
1	2.5612210	-0.5430250	-0.7930410
Method-05-AMOEBA09-Single-NMA			
6	1.8171140	-0.5781820	0.0000070
1	1.7125020	-1.6846820	0.0002260
1	2.4044280	-0.2860200	0.8979030
1	2.4042670	-0.2863490	-0.8981020
6	0.4932670	0.1648050	0.0000000
8	0.4643280	1.3839520	-0.0000080
7	-0.6377130	-0.6180240	-0.0000050
1	-0.5754400	-1.6202660	-0.0000720
6	-1.9919330	-0.0916830	0.0000070
1	-2.0010150	1.0208390	-0.0015740
1	-2.5535540	-0.4305890	-0.8978850
1	-2.5525060	-0.4280170	0.8995180
Method-06-PBFF-Single-NMA			
6	1.8192170	-0.5644000	-0.0000840
1	1.6596930	-1.6483920	0.0001700
1	2.4028470	-0.3027210	0.8887120
1	2.4025330	-0.3030920	-0.8891940
6	0.4854770	0.1716280	0.0000010
8	0.4271210	1.3959900	0.0001240
7	-0.6246210	-0.6306980	-0.0000700
1	-0.4996480	-1.6330390	-0.0001710
6	-1.9773200	-0.1022470	0.0000410
1	-1.9506710	0.9933760	-0.0011830
1	-2.5122780	-0.4455220	-0.8919330
1	-2.5113440	-0.4435350	0.8933400

Table S4 Vibration frequencies of optimized monomers obtained using various methods

Water							
Assignment	Mode Nr.	EXP.[1]	MP2/ cc-pVTZ	B3LYP/ cc-pVTZ	M06-2X/ cc-pVTZ	AMOEBA09	PBFF
0-H stretch	3	3756	3975	3901	3978	3753	3918
H-CH, stretch	2	3657	3855	3800	3874	3655	3855
CH, asyrn stretch	1	1595	1652	1639	1624	1592	1624
RMSE of vibration frequency			174	120	180	3	149

[1] Results from the reference (T. A. Halgren, *J. Comput. Chem*., 1996, **17**, 553–586.)

Methanol							
Assignment	Mode Nr.	EXP.[2]	MP2/ cc-pVTZ	B3LYP/ cc-pVTZ	M06-2X/ cc-pVTZ	AMOEBA09	PBFF
O-H stretch	12	3682	3882	3830	3911	3909	3847
H-CH, stretch	11	2999	3182	3101	3132	3170	3089
CH, asyrn stretch	10	2970	3120	3027	3083	3165	3083
CH, sym stretch	9	2844	3052	2985	3027	3045	2970
H-C-H scissor	8	1478	1537	1512	1523	1541	1685
CH, twist	7	1465	1522	1496	1504	1526	1533
CH, umbrella bend	6	1454	1497	1482	1489	1517	1521
C-O-H bend (+ CH, rock)	5	1334	1388	1376	1380	1379	1372
CH, rock	4	1145	1188	1171	1184	1201	1180
C-O stretch	3	1074	1105	1084	1120	1101	1149
CH, rock (+ COH bend)	2	1034	1070	1048	1075	1083	1063
C-O torsion	1	272	310	308	335	287	336
RMSE of vibration frequency			114	72	105	122	104

[2] Results from the reference (A. Serrallach, R. Meyer and H. Günthard, *J. Mol. Spectrosc.*,1974, **52**, 94–129.)

Methylamine							
Assignment	Mode Nr.	EXP.[3,4]	MP2/ cc-pVTZ	B3LYP/ cc-pVTZ	M06-2X/ cc-pVTZ	AMOEBA09	PBFF
NH, asym stretch	15	3424	3632	3567	3614	3634	3608
NH, sym stretch	14	3360	3539	3492	3533	3569	3542
CH, asym stretch	13	2985	3171	3087	3123	3167	3159
CH, sym stretch	12	2962	3132	3054	3087	3161	3151
H-CH, stretch	11	2820	3042	2960	3012	3058	3059
H-N-H scissor	10	1623	1666	1665	1656	1661	1630
H-CH, wag	9	1476	1541	1519	1525	1522	1552
H-C-H scissor	8	1474	1520	1498	1505	1515	1434
CH, umbrella bend	7	1430	1466	1459	1458	1493	1426
NH, twist	6	1337	1360	1350	1346	1233	1204
H-CH, rock in Cs plane	5	1130	1191	1172	1177	1204	1166
N-C stretch	4	1044	1083	1054	1087	1065	1070
CH, twist	3	995	983	975	968	1044	980
NH, wag	2	780	868	841	846	854	839
C-N torsion	1	264	311	300	297	310	381
RMSE of vibration frequency			119	77	101	130	125

[3] Results from the reference (H. Wolff and H. Ludwig, Ber. Bunsenges. *Phys. Chem*., 1966, **70**, 474–485.)

[4] Results from the reference (A. Y. Hirakawa, M. Tsuboi and T. Shimanouchi, *J. Chem.Phys*., 1972, **57**, 1236–1247.)

N-methylacetamide							
Assignment	Mode Nr.	EXP.[5]	MP2/ cc-pVTZ	B3LYP/ cc-pVTZ	M06-2X/ cc-pVTZ	AMOEBA09	PBFF
NH s	30	3498	3698	3646	3693	3680	3650
CCH_3 as	29	3008	3202	3140	3169	2985	3097
CCH_3 as	28	3008	3189	3116	3157	2980	3097
NCH_3 as	27	2973	3188	3114	3156	2977	3094
NCH_3 as	26	2973	3155	3069	3117	2973	3094
CCH_3 ss	25	2958	3092	3043	3073	2886	2992
NCH_3 ss	24	2915	3079	3024	3057	2884	2990
Amide I	23	1707	1770	1754	1803	1680	1660
Amide II	22	1511	1578	1561	1576	1649	1638
NCH_3 ab	21	1472	1523	1503	1513	1541	1557
NCH_3 ab	20	1446	1514	1497	1505	1460	1488
CCH_3 ab	19	1432	1501	1488	1492	1454	1486
CCH_3 ab	18	1432	1487	1472	1476	1440	1480
NCH_3 sb	17	1419	1444	1440	1445	1418	1462
CCH_3 sb	16	1370	1402	1399	1399	1417	1456
Amide III	15	1266	1285	1269	1284	1299	1277
NCH_3 r CN s NH ipb	14	1168	1177	1169	1179	1113	1157
NCH_3 r	13	–	1165	1153	1160	1080	1137
NCH_3 s CCH_3 r	12	1089	1128	1102	1128	1050	1045
CCH_3 r	11	1037	1056	1054	1059	934	1024
CCH_3 r CC s NCH_3 s	10	980	1005	993	1007	920	960
NCH_3 r CCH_3 s CO–NH s	9	857	878	866	885	798	790
CO ipb CC s	8	658	638	635	641	607	596
CO opb CCH_3 r	7	619	630	622	635	597	587

CO NH opb	6	439	434	452	443	472	430
CNC d CO ipb CCH_3 r	5	429	426	433	439	340	422
CNC d	4	279	290	287	298	306	259
CNC d NH opb	3	–	161	167	171	237	147
CCH_3 d	2	–	48	71	85	87	77
NCH_3 d	1	–	20	54	48	27	56
RMSE of vibration frequency			101	66	89	63	71

Notes: In the vibrations assignment column here and thereafter s is for stretch, as = asymmetric stretch, ss = symmetric stretch, d = deformation, r = rocking, ab = asymmetric bend, sb = symmetric bend, ipb = in-plane bend, opb = out-of-plane bend.

[5] The experimental IR spectra were obtained from reference (N. Tukachev, V. Bataev and I. Godunov, *Comput. Theor. Chem*.,2017, **1113**, 82–93.)

Table S5 Using different methods to predict the interaction energies of the equilibrium structure in S66×8 and S66 data set

hydrogen bond dimer	CCSD(T)/CBS		MP2/cc-pVTZ		B3LYP-D3/cc-pVTZ		M06-2X-D3/cc-pVTZ		AMOEBA09		PBFF	
	S66	S66×8	S66	S66×8	S66	S66×8	S66	S66×8	S66	S66×8	S66	S66×8
water ··water	-5.01	-4.89	-4.47	-4.49	-5.24	-5.16	-5.08	-5.07	-5.15	-5.08	-5.20	-5.03
water ··methanol	-5.70	-5.57	-4.85	-4.88	-5.69	-5.85	-5.47	-5.46	-5.70	-5.68	-5.36	-5.25
water ··methylamine	-7.04	-6.88	-6.03	-6.06	-7.09	-7.47	-6.53	-6.54	-8.45	-8.25	-6.52	-6.26
water ··NMA	-8.22	-8.08	-6.85	-6.88	-8.19	-8.48	-8.26	-8.22	-8.11	-8.05	-8.18	-8.07
methanol ··methanol	-5.85	-5.75	-5.12	-5.14	-5.99	-6.00	-5.64	-5.63	-5.50	-5.52	-6.12	-6.05
methanol ··methylamine	-7.67	-7.54	-6.87	-6.88	-8.01	-8.11	-7.38	-7.37	-7.99	-7.95	-7.62	-7.46
methanol ··NMA	-8.34	-8.22	-7.17	-7.18	-8.66	-8.70	-8.40	-8.38	-8.08	-8.07	-8.41	-8.36
methanol ··water	-5.09	-5.00	-4.66	-4.67	-5.44	-5.21	-5.22	-5.20	-4.81	-4.81	-5.71	-5.60
methylamine ··methanol	-3.11	-3.04	-2.55	-2.57	-3.32	-3.30	-2.81	-2.80	-2.90	-2.89	-3.18	-3.15
methylamine ··methylamine	-4.22	-4.15	-3.65	-3.66	-4.27	-4.26	-4.16	-4.14	-3.02	-3.13	-4.10	-4.07
methylamine ··NMA	-5.48	-5.41	-4.64	-4.65	-5.67	-5.67	-5.67	-5.62	-4.72	-4.77	-5.82	-5.82
methylamine ··water	-7.40	-7.25	-6.47	-6.49	-7.43	-7.72	-7.18	-7.17	-7.14	-7.17	-6.66	-6.48
NMA ··methanol	-6.28	-6.18	-5.63	-5.63	-6.40	-6.30	-6.22	-6.21	-6.12	-6.17	-6.51	-6.48
NMA ··methylamine	-7.56	-7.45	-7.00	-7.00	-7.83	-7.75	-7.38	-7.38	-7.46	-7.49	-7.59	-7.54
NMA ··NMA	-8.72	-8.63	-7.65	-7.65	-8.97	-9.02	-8.59	-8.58	-9.02	-9.01	-8.43	-8.41
NMA ··water	-5.20	-5.12	-4.86	-4.87	-5.48	-5.15	-5.37	-5.36	-5.09	-5.10	-5.89	-5.82

Table S6 The hydrogen bond length(Å) of 16 optimized hydrogen bond complexes by different methods

hydrogen bond dimer	Reference	MP2/cc-pVTZ	B3LYP-D3/cc-pVTZ	M06-2X-D3/cc-pVTZ	AMOEBA09	PBFF
water···water	1.963	1.946	1.943	1.943	1.936	1.838
water···methanol	1.919	1.901	1.907	1.919	1.900	1.858
water···methylamine	1.962	1.925	1.921	1.939	1.891	1.874
water···NMA	1.862	1.863	1.873	1.863	1.825	1.847
methanol···methanol	1.906	1.875	1.886	1.917	1.915	1.868
methanol···methylamine	1.939	1.887	1.895	1.913	1.909	1.861
methanol···NMA	1.855	1.830	1.846	1.863	1.838	1.869
methanol···water	1.952	1.918	1.920	1.926	1.953	1.852
methylamine···methanol	2.200	2.186	1.895	1.908	1.909	2.197
methylamine···methylamine	2.244	2.194	2.211	2.223	2.248	2.204
methylamine···NMA	2.204	2.209	2.255	2.228	2.182	2.231
methylamine···water	1.941	1.925	1.921	1.930	1.892	1.873
NMA···methanol	1.990	1.955	1.986	2.006	2.055	2.004
NMA···methylamine	2.049	2.004	2.023	2.061	2.046	2.012
NMA···NMA	1.947	1.909	1.932	1.970	1.951	2.003
NMA···water	2.053	2.020	2.035	2.046	2.108	1.998
RMSE		0.032	0.081	0.075	0.080	0.061

Table S7 Interaction energies(kcal·mol-1) of 16 optimized hydrogen bond complexes by using different methods

hydrogen bond dimer	Reference	MP2/cc-pVTZ	B3LYP-D3/cc-pVTZ	M06-2X-D3/cc-pVTZ	AMOEBA09	PBFF
water···water	-5.01	-4.40	-5.24	-5.09	-4.99	-5.59
water···methanol	-5.70	-4.76	-5.66	-5.57	-5.89	-5.84
water···methylamine	-7.04	-6.14	-7.30	-6.98	-8.53	-7.02
water···NMA	-8.22	-7.39	-8.06	-8.38	-8.22	-8.19
methanol···methanol	-5.85	-5.11	-6.03	-6.04	-5.78	-6.58
methanol···methylamine	-7.67	-6.96	-8.12	-7.68	-8.35	-8.29
methanol···NMA	-8.34	-7.18	-8.65	-8.55	-8.25	-8.68
methanol···water	-5.09	-4.58	-5.44	-5.22	-4.83	-6.18
methylamine···methanol	-3.11	-2.44	-8.12	-7.64	-8.35	-3.35
methylamine···methylamine	-4.22	-3.61	-4.26	-4.22	-3.76	-4.37
methylamine···NMA	-5.48	-4.62	-5.61	-5.88	-5.12	-6.06
methylamine···water	-7.40	-6.14	-7.30	-7.31	-8.53	-7.34
NMA···methanol	-6.28	-5.55	-6.36	-6.35	-6.42	-6.82
NMA···methylamine	-7.56	-6.97	-7.81	-7.41	-8.10	-8.09
NMA···NMA	-8.72	-7.80	-9.06	-8.63	-9.27	-9.41
NMA···water	-5.20	-4.60	-5.25	-5.25	-5.16	-6.11
RMSE		0.82	1.27	1.14	1.43	0.55

Table S8 Optimized trimer coordinates obtained via the MP2/cc-pVDZ method

Trimer01-Water-Water-Water			
8	0.6066670	1.4760580	0.1196780
1	-0.3080240	1.1242240	0.1058040
1	0.6544300	1.9623920	-0.7139190
8	0.9849240	-1.2621250	-0.1068630
1	1.1361880	-0.2944880	-0.0642520
1	1.3251480	-1.5622030	0.7460070
8	-1.5848570	-0.2042980	-0.0931350
1	-2.0270390	-0.4752390	0.7217180
1	-0.8345700	-0.8317660	-0.1527990
Trimer02-Water-Water-Methanol			
8	-1.4534410	-1.2940390	0.2111520
1	-0.5254930	-1.1749520	-0.0837160
1	-1.8648050	-1.7095660	-0.5578960
8	-1.1506020	1.4596950	0.1328360
1	-1.7405240	1.8301310	-0.5363700
1	-1.5251030	0.5668760	0.2866760
8	0.9272550	-0.1614740	-0.6242000
1	0.3375680	0.6103050	-0.4860760
6	1.9823900	-0.0247820	0.3186050
1	2.6147640	-0.9226260	0.2466450
1	2.6127180	0.8576170	0.1037700
1	1.6108380	0.0574520	1.3570400
Trimer03-Water-Water-Methylamine			
8	0.9911740	1.4835890	0.3122320
1	0.0501150	1.2676520	0.1031560
1	1.2323640	2.0893290	-0.4007010
8	1.8476800	-1.1316250	-0.2794080
1	1.6520680	-0.1907600	-0.0942840
1	2.1440610	-1.4361860	0.5875520
7	-1.5272610	0.4297150	-0.3750080
1	-1.4881660	0.2327020	-1.3791270
1	-2.4415960	0.8653030	-0.2281660
6	-1.4742250	-0.8539070	0.3515990
1	-1.5786810	-0.6537860	1.4297880
1	-2.2601630	-1.5735310	0.0556340
1	-0.4846590	-1.3009920	0.1790170
Trimer04-Water-Water-NMA			
8	2.3031300	1.4631570	-0.3031610
1	2.3479480	2.1980570	0.3225880
1	1.3344710	1.3516210	-0.4159360
8	2.8982800	-0.9848460	0.9138420
1	3.4915390	-1.3544090	0.2472230

1	2.7500470	-0.0849830	0.5562020
6	0.0648280	-1.2851090	-0.8456260
1	-0.4391590	-2.2636600	-0.8474850
1	0.9737290	-1.3359840	-0.2231420
1	0.3723790	-1.0375940	-1.8742350
6	-0.8144870	-0.1645910	-0.3321790
8	-0.4300630	1.0134210	-0.2944830
7	-2.0583230	-0.5306440	0.0840500
1	-2.3040520	-1.5122030	0.0462330
6	-3.0097360	0.4169010	0.6357280
1	-2.5475250	1.4111610	0.5750940
1	-3.9483390	0.4173780	0.0577990
1	-3.2371830	0.1880650	1.6901840
Trimer05-Water-Methanol-Methanol			
8	0.0537340	1.9472980	0.0305600
1	0.6605400	1.3066100	0.4589070
1	0.6194560	2.3788770	-0.6228390
8	-1.1555730	-0.4485640	-0.5011400
1	-0.9265660	0.5053010	-0.4996940
6	-2.4048180	-0.5681660	0.1669830
1	-2.6370390	-1.6403910	0.2521890
1	-2.3816540	-0.1344250	1.1839620
1	-3.2201340	-0.0833950	-0.4004920
8	1.2878740	-0.4239610	0.7272200
1	0.4012670	-0.6989300	0.4063800
6	2.1829740	-0.7318320	-0.3322480
1	3.1906160	-0.4136600	-0.0236480
1	2.2152470	-1.8152560	-0.5470880
1	1.9210510	-0.2029290	-1.2692010
Trimer06-Water-Methanol-Methylamine			
8	-0.0078010	1.8676820	-0.0468080
1	0.7403570	1.3056390	0.2721410
1	0.3624850	2.2875180	-0.8343900
8	-1.5582590	-0.3300800	-0.6899040
1	-1.0936810	0.5198980	-0.5375750
6	-2.2277050	-0.6132910	0.5206290
1	-2.7539210	-1.5743870	0.4033250
1	-1.5380690	-0.7114540	1.3847130
1	-2.9812950	0.1549870	0.7831220
7	1.8821230	-0.0855250	0.6486960
1	1.5077180	-0.5608710	1.4748160
1	2.8734890	0.0586460	0.8577880
6	1.7484770	-0.9845920	-0.5133730
1	2.2073820	-0.5005550	-1.3904400
1	2.2268120	-1.9725990	-0.3794700

1	0.6777040	-1.1216660	-0.7247400
Trimer07-Water-Methanol-NMA			
8	-1.5623820	1.8704420	-0.2977230
1	-0.6163090	1.6239730	-0.3959600
1	-1.5135840	2.6310160	0.2963520
8	-2.5473890	-0.4006150	0.9058110
1	-2.2275450	0.4578190	0.5540890
6	-3.5928980	-0.7887050	0.0368180
1	-3.9990470	-1.7472290	0.3984450
1	-4.4231010	-0.0558620	0.0171770
1	-3.2519210	-0.9371310	-1.0076480
6	0.2318060	-1.1687130	-0.7482280
1	0.5887850	-2.2098590	-0.7414780
1	-0.0769250	-0.9015380	-1.7715870
1	-0.6532260	-1.0746690	-0.0963830
6	1.2819530	-0.1770450	-0.2949620
8	1.0703800	1.0445860	-0.2669340
7	2.4776380	-0.7092900	0.0797820
1	2.5827080	-1.7158570	0.0465840
6	3.5791810	0.1023880	0.5650090
1	3.2556410	1.1504590	0.5130370
1	3.8297390	-0.1473830	1.6093240
1	4.4761920	-0.0315520	-0.0614860
Trimer08-Water-Methylamine-Methylamine			
8	0.3631680	2.0494470	-0.0173230
1	0.9431290	1.3232570	0.3097840
1	0.7286910	2.2093420	-0.8972100
7	-1.5730630	-0.2824420	-0.6180820
1	-2.1270840	-0.0995180	-1.4585390
1	-1.0657850	0.5930970	-0.4388200
6	-2.4938150	-0.5156560	0.4979830
1	-1.9115130	-0.6536840	1.4243410
1	-3.2262430	0.2953690	0.6877920
1	-3.0608050	-1.4467640	0.3292490
7	1.8403360	-0.2815570	0.6882150
1	1.3147290	-0.7504230	1.4312010
1	2.8062420	-0.2566830	1.0256460
6	1.7634410	-1.1087920	-0.5294960
1	2.3250830	-0.6098410	-1.3362900
1	2.1732740	-2.1298860	-0.4115210
1	0.7062640	-1.1751610	-0.8289010
Trimer09-Water-Methylamine-NMA			
8	1.2702380	-0.6435910	1.9638720
1	1.7362410	-0.6705920	1.0932800
1	1.3148410	-1.5568910	2.2741740

7	2.1118570	-0.2990100	-0.6837510
1	1.2031050	0.1519960	-0.8375810
1	2.1602050	-1.0454250	-1.3822640
6	3.1820930	0.6757470	-0.9430000
1	4.1605810	0.1935890	-0.7910380
1	3.1660900	1.1123930	-1.9591490
1	3.1002310	1.4976230	-0.2146850
6	-1.2035420	-1.7716210	-0.3112970
1	-0.9712150	-2.0838390	-1.3423240
1	-2.0277780	-2.4101070	0.0437450
1	-0.3216690	-1.9124390	0.3287680
6	-1.6798540	-0.3244550	-0.3329100
8	-2.6575700	0.0412040	-0.9816130
7	-0.8964180	0.5384380	0.3951330
1	-0.2628070	0.1336290	1.0926530
6	-1.3460280	1.9080700	0.5836220
1	-1.6481930	2.3295340	-0.3861400
1	-2.2151700	1.9747510	1.2629670
1	-0.5198890	2.5024350	1.0013620
Trimer10-Water-NMA-NMA			
8	-0.1675850	2.1344160	-1.2625440
1	-0.1390090	2.1568130	-2.2282940
1	0.7110740	1.7609040	-1.0397960
6	-0.6922880	-1.3711860	-0.9668730
1	-0.1515420	-0.5033440	-1.3694460
1	-0.9442890	-2.0727350	-1.7770220
1	-0.0364880	-1.9048490	-0.2590600
6	-1.9733340	-0.9842650	-0.2374070
8	-2.7843840	-1.8203500	0.1605240
7	-2.1203590	0.3592470	-0.0262790
1	-1.4960930	1.0127200	-0.5101790
6	-3.3346810	0.8604500	0.5904160
1	-3.5774930	0.2538940	1.4758080
1	-3.1762930	1.9060640	0.8935390
1	-4.2016860	0.8132840	-0.0933950
6	3.3589660	-1.2647700	-0.3400240
1	3.7234820	-1.8266500	0.5334350
1	4.2140120	-0.8774920	-0.9125950
1	2.7964400	-1.9484410	-0.9969300
6	2.4591570	-0.1017620	0.0302310
8	2.2153750	0.8069520	-0.7762420
7	1.9409560	-0.1307620	1.2844090
1	2.1194870	-0.9432580	1.8625610
6	1.0099090	0.8856860	1.7561760
1	1.3590560	1.8738820	1.4216360

1	-0.0084760	0.7204410	1.3686070
1	0.9900100	0.8663180	2.8552040
Trimer11-Methanol-Methanol-Methanol			
8	-0.7864650	1.6398200	-0.7075830
1	-0.0288220	1.8609310	-1.2679840
6	-0.4186980	1.9971430	0.6349420
1	-1.3073360	1.8178740	1.2574010
1	0.4129010	1.3758310	1.0042890
1	-0.1596270	3.0676700	0.7060890
8	-0.8048600	-1.1079010	-0.4399080
1	-0.9142220	-0.1575010	-0.6529940
6	-1.9987110	-1.5274340	0.2046300
1	-1.8783570	-2.5877000	0.4731030
1	-2.2025040	-0.9589320	1.1320280
1	-2.8779020	-1.4379170	-0.4596150
8	1.6433380	-0.6512830	0.7675900
1	0.7700700	-0.9650930	0.4567040
6	2.3991700	-0.4523570	-0.4084480
1	3.4026040	-0.1046680	-0.1156620
1	2.5181170	-1.3776040	-1.0046890
1	1.9584060	0.3179150	-1.0762070
Trimer12-Methanol-Methanol-Methylamine			
8	0.2957150	1.2517080	-0.5312610
1	0.9954300	0.5596840	-0.4098590
6	0.7584580	2.4106250	0.1405490
1	-0.0409310	3.1669740	0.1069990
1	1.0009350	2.2190480	1.2042570
1	1.6551040	2.8407770	-0.3454400
8	-1.6484300	-0.2637900	0.7125800
1	-1.0025220	0.3551300	0.3108270
6	-2.6205890	-0.4854850	-0.2892500
1	-3.3752750	-1.1791340	0.1155220
1	-3.1437180	0.4439220	-0.5891350
1	-2.1978030	-0.9432490	-1.2062800
7	1.9805980	-0.8587660	0.0979650
1	2.1694410	-0.7687790	1.1005500
1	2.8943260	-1.0413200	-0.3255270
6	1.1006710	-2.0260670	-0.1104240
1	0.9579200	-2.1704550	-1.1929870
1	1.4937530	-2.9675080	0.3158480
1	0.1196370	-1.8015070	0.3336640
Trimer13-Methanol-Methanol-NMA			
8	-1.2737460	1.2657760	-0.5253710
1	-0.3141880	1.0894870	-0.6313560
6	-1.3667720	2.5767480	0.0147200

1	-2.4258190	2.7718600	0.2435000
1	-0.7819010	2.6883310	0.9463810
1	-1.0210290	3.3404370	-0.7060020
8	-2.2542860	-0.8319940	0.9462800
1	-1.9061740	-0.0301130	0.5007910
6	-3.3331110	-1.2577350	0.1378010
1	-3.7663650	-2.1620990	0.5950310
1	-4.1368030	-0.4987780	0.0650690
1	-3.0218650	-1.5151640	-0.8946830
6	3.3928450	0.2516210	0.7608040
1	3.9797970	-0.6590700	0.9538830
1	3.1475760	0.7344850	1.7202850
1	3.9989520	0.9611440	0.1782210
6	2.1034040	-0.0108770	0.0053350
8	1.4311300	0.9228190	-0.4560680
7	1.7554110	-1.3132570	-0.1383210
1	2.2978160	-2.0113000	0.3559090
6	0.5099400	-1.7129300	-0.7835190
1	-0.3612900	-1.5727580	-0.1231950
1	0.3719020	-1.1067910	-1.6916140
1	0.5888920	-2.7706420	-1.0735470
Trimer14-Methanol-Methylamine-Methylamine			
8	0.0441390	1.5757320	-0.7214660
1	0.7153400	0.9738040	-0.3142110
6	-0.3609530	2.4457180	0.3156490
1	-1.1563010	3.1007280	-0.0752450
1	-0.7700100	1.9075670	1.1956600
1	0.4630300	3.0949420	0.6729000
7	-1.2795530	-1.1837440	-0.4226550
1	-1.3994390	-1.6927980	-1.3021380
1	-1.0884240	-0.2128830	-0.7015460
6	-2.5451140	-1.2240150	0.3179840
1	-2.4418170	-0.6319090	1.2419800
1	-3.4236010	-0.8330340	-0.2330490
1	-2.7697450	-2.2611360	0.6173000
7	1.5234150	-0.4470410	0.5142080
1	0.6746790	-1.0195470	0.3912300
1	1.6852930	-0.3984400	1.5232080
6	2.6623400	-1.1173340	-0.1241340
1	3.5697530	-0.5022180	-0.0110650
1	2.8818380	-2.1278190	0.2718700
1	2.4616260	-1.2138310	-1.2030310
Trimer15-Methanol-Methylamine-NMA			
8	-2.3916520	-1.6460470	0.1219050
1	-2.7910480	-2.5212900	0.2134450

6	-2.5820290	-1.2473150	-1.2365350
1	-2.1764200	-0.2285150	-1.3258790
1	-2.0528730	-1.9154440	-1.9434100
1	-3.6533400	-1.2268700	-1.5128310
7	-1.3914990	1.8767520	-0.5252750
1	-1.3439340	2.8489200	-0.8410200
1	-0.4157280	1.6319310	-0.3239450
6	-2.1428290	1.8379150	0.7349490
1	-2.2378130	0.7906950	1.0645890
1	-1.7014490	2.4257010	1.5663610
1	-3.1652660	2.2168900	0.5660520
6	3.3225810	-0.1272820	-1.0739080
1	3.9109130	-1.0252080	-0.8286400
1	3.9794320	0.7544560	-1.0706190
1	2.9117590	-0.2351150	-2.0913230
6	2.1767810	0.1211020	-0.1050180
8	1.6338000	1.2247850	-0.0096400
7	1.8053010	-0.9603880	0.6393450
1	2.2191290	-1.8576160	0.4162490
6	0.6550120	-0.9206500	1.5313040
1	0.5325570	0.1180030	1.8690450
1	-0.2749700	-1.2430390	1.0340090
1	0.8481550	-1.5605740	2.4065570
Trimer16-Methanol-NMA-NMA			
8	-2.9148490	0.2595960	0.1989240
1	-3.7348330	0.7585730	0.3177520
6	-3.1384850	-0.6764470	-0.8642930
1	-2.2068080	-1.2475000	-0.9789520
1	-3.9623410	-1.3705470	-0.6197590
1	-3.3705800	-0.1654600	-1.8161910
6	0.0999030	1.3049330	-1.8600230
1	-0.9375040	1.6492460	-1.9996890
1	0.1193200	0.2093980	-1.9863720
1	0.7509090	1.7699790	-2.6135030
6	0.6219570	1.6526120	-0.4764540
8	1.7939710	1.9739740	-0.2548410
7	-0.3029660	1.5629660	0.5223830
1	-1.2300680	1.1817140	0.3282710
6	0.1074340	1.7777790	1.8945740
1	0.5486300	2.7799260	2.0187970
1	-0.7720780	1.6849540	2.5488060
1	0.8693200	1.0432340	2.2120220
6	-0.3315600	-1.7512480	1.5487480
1	0.2448440	-1.5190200	2.4575120
1	-0.7304240	-2.7750630	1.6282280

1	-1.1869610	-1.0626530	1.4705590
6	0.4861140	-1.6580070	0.2710290
8	-0.0091120	-1.9133500	-0.8332790
7	1.7939880	-1.3113340	0.4368500
1	2.0943940	-1.0084150	1.3557360
6	2.7076690	-1.1382460	-0.6819760
1	2.8923960	-0.0701030	-0.8780750
1	3.6606490	-1.6512970	-0.4748530
1	2.2357100	-1.5983940	-1.5609780
Trimer17-Methylamine-Methylamine-Methylamine			
7	1.4107880	-1.1015140	-0.6191510
1	1.2999660	-0.0779750	-0.6747450
1	1.9804240	-1.3583170	-1.4293310
6	2.1564290	-1.4271460	0.6001980
1	2.2860410	-2.5194320	0.6823450
1	3.1600120	-0.9617430	0.6776230
1	1.5725280	-1.1014530	1.4770380
7	-1.6593110	-0.6710060	-0.6191440
1	-2.1665510	-1.0358660	-1.4293380
1	-0.7175320	-1.0868990	-0.6747320
6	-2.3142060	-1.1539100	0.6001830
1	-1.7401360	-0.8112270	1.4770380
1	-3.3248920	-0.7198620	0.6823630
1	-2.4131140	-2.2557290	0.6775360
7	0.2485590	1.7725200	-0.6191670
1	-0.5824460	1.1647810	-0.6747580
1	0.1861210	2.3942640	-1.4293290
6	0.1577540	2.5810580	0.6002020
1	1.0388890	3.2394570	0.6823450
1	-0.7470940	3.2174700	0.6776510
1	0.1676680	1.9125210	1.4770280
Trimer18-Methylamine-Methylamine-NMA			
7	-2.7999490	-0.8149390	-0.3511710
1	-1.9083930	-0.5394240	-0.7771250
1	-3.4607000	-0.8753680	-1.1296960
6	-3.2309110	0.2627200	0.5444110
1	-3.3458090	1.2585600	0.0696870
1	-4.1960300	-0.0021270	1.0081220
1	-2.4961930	0.3674570	1.3597380
7	0.4438900	2.7152150	-0.7734020
1	1.4193450	2.9874770	-0.9166870
1	0.3949730	1.7334380	-1.0609760
6	0.1420730	2.7777590	0.6590570
1	-0.9029370	2.4672690	0.8197620
1	0.7781200	2.1440140	1.3134640

1	0.2308310	3.8184460	1.0134470
6	0.0210510	-2.5938310	0.1591370
1	0.3920240	-3.0802000	1.0748910
1	0.1721570	-3.2803270	-0.6912300
1	-1.0572250	-2.3885900	0.2431230
6	0.7398420	-1.2908040	-0.1378240
8	0.2434600	-0.4090100	-0.8493860
7	1.9766770	-1.1648840	0.4286220
1	2.3637930	-1.9737510	0.9003920
6	2.8490890	-0.0387540	0.1449230
1	2.2201800	0.8161680	-0.1338830
1	3.4322680	0.2184840	1.0423350
1	3.5447150	-0.2497340	-0.6868520
Trimer19-Methylamine-NMA-NMA			
7	2.3499160	2.3673230	0.7077580
1	1.7601440	1.6010310	1.0474770
1	2.3911540	3.0419590	1.4754470
6	1.6619840	2.9897100	-0.4275920
1	0.6473930	3.3829310	-0.2122150
1	2.2690110	3.8226410	-0.8198210
1	1.5641370	2.2476450	-1.2372900
6	-2.4241690	-0.9636410	1.5291940
1	-1.3382770	-1.0758480	1.6657450
1	-2.8709790	-1.9474640	1.3108100
1	-2.8832230	-0.5965760	2.4602510
6	-2.7827730	-0.0071500	0.4000960
8	-3.9405010	0.3270120	0.1547760
7	-1.7119500	0.4172400	-0.3443160
1	-0.7722830	0.2381160	0.0112560
6	-1.9038880	1.4081650	-1.3868950
1	-2.8101550	1.1596290	-1.9584170
1	-2.0324650	2.4281300	-0.9805470
1	-1.0323700	1.4014590	-2.0587140
6	3.3325850	-0.8384850	0.4233840
1	4.0062870	-1.3508900	-0.2804840
1	3.5492410	-1.1912200	1.4456490
1	3.5052790	0.2489210	0.3990910
6	1.8680470	-1.0940970	0.1285100
8	0.9720440	-0.3861710	0.6172290
7	1.6039470	-2.1427070	-0.6954850
1	2.3817180	-2.7325470	-0.9679740
6	0.2519300	-2.5927960	-0.9898150
1	-0.4271180	-1.7303140	-0.9594470
1	0.2251360	-3.0368370	-1.9959930
1	-0.1006530	-3.3407140	-0.2578530

Trimer20-NMA-NMA-NMA

6	-0.3130150	1.0540970	1.9275210
1	0.7759350	0.9295290	2.0135470
1	-0.7912540	0.0620770	1.9140170
1	-0.7044580	1.6014770	2.7991070
6	-0.7235770	1.7974630	0.6681180
8	-1.9021450	2.1279100	0.4584260
7	0.2932010	2.0541510	-0.1946980
1	1.2170010	1.6692530	0.0177560
6	0.0901140	2.7824680	-1.4332010
1	-0.9135690	3.2290160	-1.4013630
1	0.8422570	3.5814650	-1.5334060
1	0.1575640	2.1209120	-2.3138560
6	-2.0032860	-0.2385110	-1.9132300
1	-2.2573350	0.8011200	-1.6633920
1	-2.6217270	-0.5770810	-2.7606270
1	-0.9503340	-0.2989270	-2.2294150
6	-2.2281150	-1.1929840	-0.7508690
8	-1.8737170	-2.3755990	-0.7841510
7	-2.9016850	-0.6587980	0.3114710
1	-2.9021740	0.3579080	0.4123820
6	-3.1478740	-1.4841290	1.4800670
1	-3.6677760	-2.4071020	1.1815380
1	-2.2130440	-1.7832450	1.9895960
1	-3.7779950	-0.9242150	2.1863610
6	4.7924350	-0.6593850	0.1787810
1	5.1367240	-1.6473100	-0.1629840
1	5.1228160	-0.4999650	1.2175140
1	5.2581720	0.1234180	-0.4386220
6	3.2848030	-0.4844750	0.1191840
8	2.7645700	0.6157180	0.3500190
7	2.5796260	-1.6009990	-0.1991680
1	3.0923070	-2.4681150	-0.3083780
6	1.1252920	-1.6463910	-0.2396050
1	0.6990010	-2.0613130	0.6891660
1	0.7537580	-0.6213940	-0.3663800
1	0.7758110	-2.2611410	-1.0807480

Table S9 Interaction energies(kcal·mol^{-1}) of trimers obtained using various methods

	DLPNO-CCSD(T) Complete Basis Set	MP2 cc-pVTZ	B3LYP cc-pVTZ	B3LYP-D3 cc-pVTZ	M06-2X cc-pVTZ	M06-2X-D3 cc-pVTZ	AMOEBA09	PBFF
Trimer01	-15.30	-14.16(1.14)	-14.57(0.74)	-17.03(-1.73)	-16.91(-1.60)	-16.95(-1.64)	-16.01(-0.70)	-15.27(0.04)
Trimer02	-15.94	-14.71(1.23)	-14.49(1.45)	-17.53(-1.59)	-17.10(-1.16)	-17.22(-1.28)	-15.98(-0.04)	-15.49(0.45)
Trimer03	-15.05	-13.96(1.09)	-13.49(1.56)	-16.84(-1.79)	-15.85(-0.79)	-16.00(-0.95)	-16.76(-1.71)	-14.34(0.71)
Trimer04	-16.12	-14.55(1.57)	-14.46(1.66)	-17.91(-1.79)	-16.97(-0.86)	-17.21(-1.10)	-17.45(-1.34)	-15.30(0.82)
Trimer05	-16.37	-14.93(1.45)	-13.85(2.53)	-17.77(-1.39)	-17.20(-0.83)	-17.42(-1.05)	-15.48(0.89)	-16.42(-0.05)
Trimer06	-15.59	-14.44(1.15)	-13.14(2.44)	-17.32(-1.74)	-16.20(-0.62)	-16.46(-0.87)	-16.38(-0.79)	-15.56(0.02)
Trimer07	-17.08	-15.57(1.51)	-14.66(2.42)	-18.86(-1.78)	-17.78(-0.70)	-18.13(-1.05)	-17.24(-0.16)	-16.34(0.74)
Trimer08	-12.26	-11.17(1.10)	-9.69(2.57)	-13.64(-1.38)	-12.43(-0.17)	-12.72(-0.46)	-13.97(-1.71)	-12.02(0.25)
Trimer09	-15.33	-14.36(0.97)	-11.56(3.77)	-16.97(-1.64)	-15.86(-0.54)	-16.33(-1.01)	-16.26(-0.94)	-14.59(0.73)
Trimer10	-17.27	-15.67(1.60)	-11.62(5.65)	-19.07(-1.80)	-17.91(-0.64)	-18.64(-1.36)	-17.47(-0.20)	-16.63(0.64)
Trimer11	-13.84	-12.50(1.34)	-10.15(3.69)	-15.32(-1.48)	-14.17(-0.33)	-14.53(-0.69)	-13.67(0.17)	-14.40(-0.55)
Trimer12	-16.83	-15.81(1.02)	-13.73(3.10)	-18.52(-1.70)	-16.92(-0.09)	-17.31(-0.48)	-16.46(0.37)	-16.94(-0.11)
Trimer13	-17.59	-16.13(1.46)	-13.98(3.61)	-19.34(-1.74)	-17.86(-0.27)	-18.42(-0.83)	-17.00(0.59)	-16.68(0.91)
Trimer14	-15.09	-14.15(0.95)	-11.85(3.24)	-16.47(-1.37)	-14.98(0.11)	-15.40(-0.31)	-15.43(-0.34)	-15.72(-0.62)
Trimer15	-8.20	-7.24(0.95)	-4.02(4.17)	-9.22(-1.03)	-7.49(0.71)	-8.15(0.05)	-9.07(-0.87)	-7.32(0.88)
Trimer16	-15.89	-14.13(1.76)	-5.86(10.03)	-17.28(-1.39)	-16.05(-0.15)	-17.03(-1.14)	-15.86(0.04)	-15.45(0.44)
Trimer17	-11.68	-11.03(0.65)	-8.37(3.31)	-12.77(-1.09)	-11.23(0.45)	-11.71(-0.03)	-12.07(-0.40)	-12.21(-0.53)
Trimer18	-9.03	-7.78(1.25)	-4.02(5.00)	-10.04(-1.01)	-8.81(0.22)	-9.50(-0.47)	-8.92(0.10)	-9.77(-0.74)
Trimer19	-13.62	-12.28(1.34)	-7.49(6.14)	-14.82(-1.20)	-13.33(0.29)	-14.29(-0.67)	-13.54(0.08)	-14.80(-1.18)
Trimer20	-21.12	-19.11(2.01)	-10.43(10.69)	-22.69(-1.57)	-21.64(-0.52)	-22.95(-1.84)	-19.97(1.15)	-22.79(-1.67)
Root Mean Square Error		1.31	4.64	1.53	0.67	0.98	0.82	0.72
Mean Absolute Error		1.28	3.89	1.51	0.55	0.86	0.63	0.60
Maximum Absolute Error		2.01	10.69	1.80	1.60	1.84	1.71	1.67