Molecular Mechanics Descriptions of Non-covalent Interactions: a Critical Evaluation

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Supporting Information

S22 data set: Results with infinite non-bonded cut-offs

MM2*

Complex	Monomer A (kJ/mol)	Monomer B (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	RMS geometry (Å)
Ammonia dimer	0.00	0.00	-3.00	3.00	0.1765
Water dimer	0.00	0.00	-13.35	13.35	0.2610
Formic acid dimer	-125.24	-125.24	-304.67	54.20	0.1876
Formamide dimer	-118.17	-118.17	-276.62	40.29	0.0903
Uracil dimer	-346.99	-346.99	-739.37	45.38	0.2151
Pyridoxine : aminopyridine	-103.50	-139.82	-257.34	14.03	0.4239
Adenine : thymine (WC)	95.54	-366.16	-289.66	19.04	1.6113
Methane dimer	0.00	0.00	-3.82	3.82	0.1104
Ethene dimer	1.77	1.77	-0.57	4.10	0.1502
Benzene : methane	12.56	0.00	7.53	5.03	0.0613
Benzene dimer (PD)	12.56	12.56	9.70	15.42	0.5507
Pyrazine dimer	197.66	197.66	373.50	21.83	0.3985
Uracil dimer	-346.99	-346.99	-735.33	41.34	2.3947
Indole : benzene (stacked)	12.56	60.12	53.53	19.14	0.3711
Adenine : thymine (stacked)	95.54	-366.16	-294.56	23.94	0.6744
Ethene : ethyne	1.77	-0.21	-0.43	1.99	0.1175
Bezene : water	12.56	0.00	7.90	4.66	0.2141
Benzene : ammonia	12.56	0.00	6.53	6.03	0.3772
Benzene : HCN	12.56	0.00	7.34	5.22	0.5103
Benzene dimer (t-shaped)	12.56	12.56	18.39	6.73	0.1310
Indole : benzene (t-shaped)	12.56	60.12	63.73	8.94	0.2151
Phenol dimer	15.47	15.47	14.13	16.81	2.1734

MM2* with explicit lone pairs

Complex	Monomer A (kJ/mol)	Monomer B (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	RMS geometry (Å)
Ammonia dimer	2.80	2.80	-1.26	6.87	0.8236
Water dimer	0.76	0.76	-18.87	20.39	0.3468
Formic acid dimer	30.15	30.15	0.86	59.44	0.1247
Formamide dimer	-118.17	-118.17	-276.62	40.29	0.1530
Uracil dimer	-346.99	-346.99	-739.16	45.17	0.1650
Pyridoxine : aminopyridine	-103.50	-139.82	-257.13	13.82	0.3099
Adenine : thymine (WC)	95.54	-366.16	-286.55	15.93	0.7192
Methane dimer	0.00	0.00	-3.82	3.82	0.1104
Ethene dimer	1.77	1.77	-0.57	4.10	0.1502
Benzene : methane	12.56	0.00	7.53	5.03	0.0613
Benzene dimer (PD)	12.56	12.56	9.70	15.42	0.5481
Pyrazine dimer	197.66	197.66	373.50	21.83	0.3985
Uracil dimer	-346.99	-346.99	-735.14	41.16	2.3947
Indole : benzene (stacked)	12.56	60.12	53.54	19.14	0.3709
Adenine : thymine (stacked)	95.54	-366.16	-294.51	23.90	0.6753
Ethene : ethyne	1.77	-0.21	-0.43	1.99	0.0275
Bezene : water	12.56	0.76	7.69	5.63	0.2023
Benzene : ammonia	12.56	2.80	9.04	6.32	0.2792
Benzene : HCN	12.56	0.00	7.34	5.22	0.4491
Benzene dimer (t-shaped)	12.56	12.56	18.55	6.57	0.0361
Indole : benzene (t-shaped)	12.56	60.12	63.95	8.73	0.2700
Phenol dimer	16.02	16.02	12.50	19.53	1.9942

MM3*

Complex	Monomer A (kJ/mol)	Monomer B (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	RMS geometry (Å)
Ammonia dimer	0.00	0.00	-4.86	4.86	0.2129
Water dimer	0.00	0.00	-29.75	29.75	0.3223
Formic acid dimer	-26.85	-26.85	-70.22	16.52	0.1904
Formamide dimer	-54.64	-54.64	-144.78	35.50	0.0821
Uracil dimer	-705.99	-705.99	-1429.57	17.59	0.1541
Pyridoxine : aminopyridine	-61.18	-170.89	-247.38	15.30	0.9193
Adenine : thymine (WC)	-243.05	-707.54	-965.98	15.39	0.5968
Methane dimer	0.00	0.00	-1.73	1.73	0.0274
Ethene dimer	29.32	29.32	55.42	3.21	0.2039
Benzene : methane	25.55	0.00	21.96	3.59	0.1300
Benzene dimer (PD)	25.55	25.55	40.99	10.12	0.2583
Pyrazine dimer	135.46	135.46	250.84	20.07	0.3900
Uracil dimer	-705.99	-705.99	-1427.44	15.45	0.2939
Indole : benzene (stacked)	25.55	107.05	117.08	15.52	0.4549
Adenine : thymine (stacked)	-242.69	-707.54	-982.28	32.05	0.6104

Ethene : ethyne	29.32	13.55	40.13	2.73	0.0966
Bezene : water	25.55	0.00	14.53	11.03	0.2091
Benzene : ammonia	25.55	0.00	17.68	7.87	0.3493
Benzene : HCN	25.55	0.00	12.71	12.84	0.3413
Benzene dimer (t-shaped)	25.55	25.55	43.28	7.83	0.1362
Indole : benzene (t-shaped)	25.55	107.05	123.15	9.45	1.0004
Phenol dimer	10.30	10.30	7.62	12.99	1.0836

AMBER*

Complex	Monomer A (kJ/mol)	Monomer B (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	RMS geometry (Å)
Ammonia dimer	0.00	0.00	-19.43	19.43	0.1927
Water dimer	0.00	0.00	-29.67	29.67	0.1913
Formic acid dimer	-46.69	-46.69	-138.30	44.93	0.1456
Formamide dimer	-83.24	-83.24	-229.38	62.91	0.0654
Uracil dimer	-336.61	-336.61	-716.48	43.27	0.0829
Pyridoxine : aminopyridine	-115.65	-74.66	-240.20	49.89	0.4796
Adenine : thymine (WC)	-363.92	-631.08	-1042.30	47.30	0.1759
Methane dimer	0.00	0.00	-1.29	1.29	0.0810
Ethene dimer	23.46	23.46	42.83	4.09	0.0802
Benzene : methane	29.10	0.00	25.55	3.56	0.0769
Benzene dimer (PD)	29.10	29.10	46.24	11.97	0.5473
Pyrazine dimer	106.95	106.95	186.29	27.61	0.3937
Uracil dimer	-336.61	-336.61	-709.55	36.34	0.2403
Indole : benzene (stacked)	29.10	5.13	7.48	26.76	1.5576
Adenine : thymine (stacked)	-364.94	-631.08	-1040.71	44.68	0.4272
Ethene : ethyne	23.46	18.80	37.94	4.32	0.0229
Bezene : water	29.10	0.00	5.94	23.17	0.2150
Benzene : ammonia	29.10	0.00	14.71	14.39	0.1983
Benzene : HCN	29.10	0.00	4.38	24.73	0.2984
Benzene dimer (t-shaped)	29.10	29.10	47.18	11.03	0.0768
Indole : benzene (t-shaped)	29.10	5.13	7.73	26.51	0.0856
Phenol dimer	4.02	4.02	-20.59	28.64	0.4499

AMBER* (10,12 H-bonding potential)

Complex	Monomer A (kJ/mol)	Monomer B (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	RMS geometry (Å)
Ammonia dimer	0.00	0.00	-19.43	19.43	0.1927
Water dimer	0.00	0.00	-29.92	29.92	0.1936
Formic acid dimer	-46.69	-46.69	-136.79	43.41	0.1759
Formamide dimer	-83.24	-83.24	-226.60	60.13	0.0498
Uracil dimer	-336.61	-336.61	-715.72	42.51	0.1104
Pyridoxine : aminopyridine	-115.65	-74.66	-240.58	50.27	0.5284
Adenine : thymine (WC)	-363.58	-631.08	-1041.04	46.37	0.1675
Methane dimer	0.00	0.00	-1.29	1.29	0.0810
Ethene dimer	23.46	23.46	42.83	4.09	0.0802
Benzene : methane	29.10	0.00	25.55	3.56	0.0769
Benzene dimer (PD)	29.10	29.10	46.24	11.97	0.5473
Pyrazine dimer	106.95	106.95	186.29	27.61	0.3937
Uracil dimer	-336.61	-336.61	-709.34	36.12	0.2511
Indole : benzene (stacked)	29.10	5.13	7.48	26.76	1.5577
Adenine : thymine (stacked)	-364.61	-631.08	-1040.29	44.60	0.4276
Ethene : ethyne	23.46	18.80	37.94	4.32	0.0229
Bezene : water	29.10	0.00	5.94	23.17	0.2150
Benzene : ammonia	29.10	0.00	14.71	14.39	0.1983
Benzene : HCN	29.10	0.00	4.38	24.73	0.2987
Benzene dimer (t-shaped)	29.10	29.10	47.18	11.03	0.0768
Indole : benzene (t-shaped)	29.10	5.13	7.73	26.51	0.0856
Phenol dimer	4.02	4.02	-20.88	28.92	0.4358

OPLS*

Complex	Monomer A (kJ/mol)	Monomer B (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	RMS geometry (Å)
Ammonia dimer	0.00	0.00	-17.05	17.05	0.1869
Water dimer	0.00	0.00	-28.61	28.61	0.1931
Formic acid dimer	-54.72	-54.72	-167.03	57.59	0.1012
Formamide dimer	-76.05	-76.05	-219.06	66.97	0.0878
Uracil dimer	-171.76	-171.76	-395.83	52.31	0.0569
Pyridoxine : aminopyridine	-68.61	-115.07	-222.96	39.28	0.2507
Adenine : thymine (WC)	-89.55	-201.01	-335.10	44.53	0.0540
Methane dimer	0.00	0.00	-2.53	2.53	0.0017
Ethene dimer	13.58	13.58	22.89	4.26	0.0638
Benzene : methane	12.60	0.00	7.91	4.69	0.1040
Benzene dimer (PD)	12.60	12.60	16.33	8.87	0.4465
Pyrazine dimer	90.01	90.01	157.21	22.81	0.3877
Uracil dimer	-171.76	-171.76	-374.08	30.56	0.2137
Indole : benzene (stacked)	12.60	-4.92	-6.98	14.66	1.0334
Adenine : thymine (stacked)	-89.55	-201.01	-331.52	40.95	0.3220

Ethene : ethyne	13.58	7.46	17.03	4.01	0.0971
Bezene : water	12.60	0.00	-3.54	16.14	0.1491
Benzene : ammonia	12.60	0.00	1.85	10.75	0.1837
Benzene : HCN	12.60	0.00	-3.23	15.83	0.1968
Benzene dimer (t-shaped)	12.60	12.60	16.19	9.01	0.0986
Indole : benzene (t-shaped)	12.60	-4.92	-18.08	25.76	0.0791
Phenol dimer	-12.39	-12.39	-62.79	38.00	0.6089

OPLSAA

Complex	Monomer A (kJ/mol)	Monomer B (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	RMS geometry (Å)
Ammonia dimer	0.00	0.00	-10.34	10.34	0.0669
Water dimer	0.00	0.00	-28.10	28.10	0.1609
Formic acid dimer	-59.29	-59.29	-171.34	52.75	0.1183
Formamide dimer	-95.49	-95.49	-248.73	57.75	0.0432
Uracil dimer	-146.10	-146.10	-344.59	52.39	0.0727
Pyridoxine : aminopyridine	0.87	-236.68	-277.48	41.67	0.2537
Adenine : thymine (WC)	-75.96	-168.26	-288.77	44.55	0.0514
Methane dimer	0.71	0.71	-0.78	2.19	0.0741
Ethene dimer	13.60	13.60	22.71	4.48	0.0519
Benzene : methane	27.95	0.71	24.21	4.45	0.0762
Benzene dimer (PD)	27.95	27.95	47.06	8.84	0.4445
Pyrazine dimer	110.54	110.54	198.33	22.74	0.3886
Uracil dimer	-146.10	-146.10	-322.26	30.06	0.2035
Indole : benzene (stacked)	27.95	10.09	13.10	24.95	1.5617
Adenine : thymine (stacked)	-75.96	-168.26	-285.50	41.27	0.3843
Ethene : ethyne	13.60	8.23	18.29	3.54	0.0189
Bezene : water	27.95	0.00	12.23	15.72	0.1332
Benzene : ammonia	27.95	0.00	18.91	9.05	0.0973
Benzene : HCN	27.95	0.00	12.88	15.08	0.2517
Benzene dimer (t-shaped)	27.95	27.95	46.91	9.00	0.1012
Indole : benzene (t-shaped)	27.95	10.09	13.33	24.72	0.0873
Phenol dimer	3.82	3.82	-25.78	33.42	0.3780

MMFF94

Complex	Monomer A (kJ/mol)	Monomer B (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	RMS geometry (Å)
Ammonia dimer	0.00	0.00	-12.65	12.65	0.0558
Water dimer	0.00	0.00	-27.65	27.65	0.2087
Formic acid dimer	-107.01	-107.01	-285.09	71.08	0.1290
Formamide dimer	-129.32	-129.32	-309.95	51.31	0.0385
Uracil dimer	-403.79	-403.79	-865.52	57.94	0.0902
Pyridoxine : aminopyridine	-24.42	-146.74	-214.06	42.90	0.1434
Adenine : thymine (WC)	-21.25	-396.10	-465.09	47.74	0.2366
Methane dimer	0.11	0.11	-1.44	1.66	0.0071
Ethene dimer	34.31	34.31	65.51	3.11	0.2418
Benzene : methane	67.89	0.11	65.41	2.60	0.2559
Benzene dimer (PD)	67.89	67.89	127.91	7.88	0.7627
Pyrazine dimer	219.82	219.82	419.32	20.32	0.3963
Uracil dimer	-403.79	-403.79	-858.64	51.06	2.3409
Indole : benzene (stacked)	67.89	63.23	110.08	21.04	1.6347
Adenine : thymine (stacked)	-21.25	-396.10	-470.55	53.20	2.2971
Ethene : ethyne	34.31	9.59	41.36	2.55	0.2069
Bezene : water	67.89	0.00	51.96	15.94	0.2130
Benzene : ammonia	67.89	0.00	57.54	10.36	0.1912
Benzene : HCN	67.89	0.00	52.57	15.32	0.3195
Benzene dimer (t-shaped)	67.89	67.89	128.34	7.45	0.2660
Indole : benzene (t-shaped)	67.89	63.23	110.18	20.94	0.1435
Phenol dimer	23.90	23.90	17.66	30.15	0.6127

MMFF94s

Complex	Monomer A (kJ/mol)	Monomer B (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	RMS geometry (Å)
Ammonia dimer	0.00	0.00	-12.65	12.65	0.0558
Water dimer	0.00	0.00	-27.65	27.65	0.2087
Formic acid dimer	-107.01	-107.01	-285.09	71.08	0.1290
Formamide dimer	-129.86	-129.86	-311.04	51.31	0.0385
Uracil dimer	-406.12	-406.12	-870.18	57.94	0.0902
Pyridoxine : aminopyridine	-25.46	-132.73	-202.56	44.36	0.1570
Adenine : thymine (WC)	-18.30	-398.43	-465.27	48.53	0.0583
Methane dimer	0.11	0.11	-1.44	1.66	0.0071
Ethene dimer	34.31	34.31	65.51	3.11	0.2418
Benzene : methane	67.89	0.11	65.41	2.60	0.2559
Benzene dimer (PD)	67.89	67.89	127.91	7.88	0.7627
Pyrazine dimer	219.82	219.82	419.32	20.32	0.3963
Uracil dimer	-406.12	-406.12	-863.30	51.06	2.3413
Indole : benzene (stacked)	67.89	63.23	110.08	21.04	1.6347
Adenine : thymine (stacked)	-18.30	-398.43	-469.79	53.06	2.4497

Ethene : ethyne	34.31	9.59	41.36	2.55	0.2069
Bezene : water	67.89	0.00	51.96	15.94	0.2130
Benzene : ammonia	67.89	0.00	57.54	10.36	0.1912
Benzene : HCN	67.89	0.00	52.57	15.32	0.3195
Benzene dimer (t-shaped)	67.89	67.89	128.34	7.45	0.2660
Indole : benzene (t-shaped)	67.89	63.23	110.18	20.94	0.1435
Phenol dimer	23.90	23.90	17.66	30.15	0.6127

S22 data set: Results with default (vdW 7 Å, electrostatic 12 Å) non-bonded cut-offs

MM2*

Complex	Monomer A (kJ/mol)	Monomer B (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	RMS geometry (Å)
Ammonia dimer	0.00	0.00	-3.00	3.00	0.1750
Water dimer	0.00	0.00	-13.35	13.35	0.2610
Formic acid dimer	-125.24	-125.24	-304.67	54.20	0.2030
Formamide dimer	-118.17	-118.17	-276.62	40.29	0.0860
Uracil dimer	-346.99	-346.99	-739.16	45.17	0.1750
Pyridoxine : aminopyridine	-103.50	-139.82	-257.13	13.82	0.3850
Adenine : thymine (WC)	95.54	-366.16	-289.42	18.80	1.3800
Methane dimer	0.00	0.00	-3.82	3.82	0.1090
Ethene dimer	1.77	1.77	-0.57	4.10	0.1490
Benzene : methane	12.56	0.00	7.53	5.03	0.0490
Benzene dimer (PD)	12.56	12.56	9.70	15.42	0.4590
Pyrazine dimer	197.66	197.66	373.50	21.83	0.3460
Uracil dimer	-346.99	-346.99	-735.14	41.16	2.0450
Indole : benzene (stacked)	12.56	60.12	53.54	19.14	0.3120
Adenine : thymine (stacked)	95.54	-366.16	-294.51	23.90	0.6380
Ethene : ethyne	1.77	-0.21	-0.43	1.99	0.1190
Bezene : water	12.56	0.00	7.90	4.66	0.1270
Benzene : ammonia	12.56	0.00	6.53	6.03	0.1900
Benzene : HCN	12.56	0.00	7.34	5.22	0.4460
Benzene dimer (t-shaped)	12.56	12.56	18.55	6.57	2.3890
Indole : benzene (t-shaped)	12.56	60.12	63.95	8.73	0.1860
Phenol dimer	15.47	15.47	14.11	16.83	1.7020

MM2* with explicit lone pairs

Complex	Monomer A (kJ/mol)	Monomer B (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	RMS geometry (Å)
Ammonia dimer	2.80	2.80	-1.26	6.87	0.4980
Water dimer	0.76	0.76	-18.87	20.39	0.1870
Formic acid dimer	30.15	30.15	0.86	59.44	0.1610
Formamide dimer	-118.17	-118.17	-276.62	40.29	0.1160
Uracil dimer	-346.99	-346.99	-739.16	45.17	0.1370
Pyridoxine : aminopyridine	-103.50	-139.82	-257.13	13.82	0.2840
Adenine : thymine (WC)	95.54	-366.16	-286.55	15.93	0.6760
Methane dimer	0.00	0.00	-3.82	3.82	0.1090
Ethene dimer	1.77	1.77	-0.57	4.10	0.1490
Benzene : methane	12.56	0.00	7.53	5.03	0.0490
Benzene dimer (PD)	12.56	12.56	9.70	15.42	0.4590
Pyrazine dimer	197.66	197.66	373.50	21.83	0.3460
Uracil dimer	-346.99	-346.99	-735.14	41.16	2.0450
Indole : benzene (stacked)	12.56	60.12	53.54	19.14	0.3120
Adenine : thymine (stacked)	95.54	-366.16	-294.51	23.90	0.6380
Ethene : ethyne	1.77	-0.21	-0.43	1.99	0.0230
Bezene : water	12.56	0.76	7.69	5.63	0.1290
Benzene : ammonia	12.56	2.80	9.04	6.32	0.1390
Benzene : HCN	12.56	0.00	7.34	5.22	0.4440
Benzene dimer (t-shaped)	12.56	12.56	18.55	6.57	2.3920
Indole : benzene (t-shaped)	12.56	60.12	63.95	8.73	0.2500
Phenol dimer	16.02	16.02	12.50	19.53	1.7270

MM3*

Complex	Monomer A (kJ/mol)	Monomer B (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	RMS geometry (Å)
Ammonia dimer	0.00	0.00	-4.86	4.86	0.2160
Water dimer	0.00	0.00	-29.75	29.75	0.3240
Formic acid dimer	-26.85	-26.85	-70.22	16.52	0.1740
Formamide dimer	-54.64	-54.64	-144.78	35.50	0.0710
Uracil dimer	-705.99	-705.99	-1429.45	17.47	1.9700
Pyridoxine : aminopyridine	-61.18	-170.89	-247.14	15.06	0.7010
Adenine : thymine (WC)	-243.05	-707.54	-967.69	17.10	0.5850
Methane dimer	0.00	0.00	-1.73	1.73	0.0210
Ethene dimer	29.32	29.32	55.42	3.21	0.2030
Benzene : methane	25.55	0.00	21.96	3.59	0.1060
Benzene dimer (PD)	25.55	25.55	41.03	10.08	0.2410
Pyrazine dimer	135.46	135.46	250.84	20.07	0.3330

Uracil dimer	-705.99	-705.99	-1427.43	15.45	0.2760
Indole : benzene (stacked)	25.55	107.05	117.13	15.48	0.4050
Adenine : thymine (stacked)	-242.69	-707.54	-982.24	32.01	0.5220
Ethene : ethyne	29.32	13.55	40.13	2.73	1.1210
Bezene : water	25.55	0.00	14.53	11.03	0.1220
Benzene : ammonia	25.55	0.00	17.68	7.87	0.1670
Benzene : HCN	25.55	0.00	12.71	12.84	0.3030
Benzene dimer (t-shaped)	25.55	25.55	43.44	7.67	0.1380
Indole : benzene (t-shaped)	25.55	107.05	123.41	9.20	0.8700
Phenol dimer	10.30	10.30	7.68	12.93	0.9090

AMBER*

Complex	Monomer A (kJ/mol)	Monomer B (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	RMS geometry (Å)
Ammonia dimer	0.00	0.00	-19.43	19.43	0.1600
Water dimer	0.00	0.00	-29.67	29.67	0.1220
Formic acid dimer	-46.69	-46.69	-138.30	44.93	0.1340
Formamide dimer	-83.24	-83.24	-229.38	62.91	0.0630
Uracil dimer	-336.61	-336.61	-716.65	43.43	1.9870
Pyridoxine : aminopyridine	-115.65	-74.66	-240.03	49.72	0.3850
Adenine : thymine (WC)	-363.92	-631.08	-1044.84	49.84	0.0850
Methane dimer	0.00	0.00	-1.29	1.29	0.0820
Ethene dimer	23.46	23.46	42.83	4.09	0.0790
Benzene : methane	29.10	0.00	25.55	3.56	0.0640
Benzene dimer (PD)	29.10	29.10	46.31	11.90	0.5020
Pyrazine dimer	106.95	106.95	186.29	27.61	0.3380
Uracil dimer	-336.61	-336.61	-709.55	36.34	0.2220
Indole : benzene (stacked)	29.10	5.13	7.65	26.59	1.2850
Adenine : thymine (stacked)	-364.94	-631.08	-1040.69	44.67	0.3300
Ethene : ethyne	23.46	18.80	37.94	4.32	0.0190
Bezene : water	29.10	0.00	5.94	23.17	0.1910
Benzene : ammonia	29.10	0.00	14.71	14.39	0.1650
Benzene : HCN	29.10	0.00	4.38	24.73	0.2760
Benzene dimer (t-shaped)	29.10	29.10	47.31	10.90	0.0780
Indole : benzene (t-shaped)	29.10	5.13	7.91	26.33	0.0840
Phenol dimer	4.02	4.02	-20.45	28.49	0.3610

AMBER* (10,12 H-bonding potential)

Complex	Monomer A (kJ/mol)	Monomer B (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	RMS geometry (Å)
Ammonia dimer	0.00	0.00	-19.43	19.43	0.1600
Water dimer	0.00	0.00	-29.92	29.92	0.1220
Formic acid dimer	-46.69	-46.69	-136.79	43.41	0.1610
Formamide dimer	-83.24	-83.24	-226.60	60.13	0.0470
Uracil dimer	-336.61	-336.61	-716.47	43.25	0.0920
Pyridoxine : aminopyridine	-115.65	-74.66	-240.41	50.10	0.4250
Adenine : thymine (WC)	-363.58	-631.08	-1043.86	49.20	0.0730
Methane dimer	0.00	0.00	-1.29	1.29	0.0820
Ethene dimer	23.46	23.46	42.83	4.09	0.0790
Benzene : methane	29.10	0.00	25.55	3.56	0.0640
Benzene dimer (PD)	29.10	29.10	46.31	11.90	0.5020
Pyrazine dimer	106.95	106.95	186.29	27.61	0.3380
Uracil dimer	-336.61	-336.61	-709.33	36.12	0.2300
Indole : benzene (stacked)	29.10	5.13	7.65	26.59	1.2850
Adenine : thymine (stacked)	-364.61	-631.08	-1040.27	44.59	0.3300
Ethene : ethyne	23.46	18.80	37.94	4.32	0.0190
Bezene : water	29.10	0.00	5.94	23.17	0.1910
Benzene : ammonia	29.10	0.00	14.71	14.39	0.1650
Benzene : HCN	29.10	0.00	4.38	24.73	0.2760
Benzene dimer (t-shaped)	29.10	29.10	47.31	10.90	0.0780
Indole : benzene (t-shaped)	29.10	5.13	7.91	26.33	0.0840
Phenol dimer	4.02	4.02	-20.73	28.78	0.3490

OPLS*

Complex	Monomer A (kJ/mol)	Monomer B (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	RMS geometry (Å)
Ammonia dimer	0.00	0.00	-17.05	17.05	0.1510
Water dimer	0.00	0.00	-28.61	28.61	0.1380
Formic acid dimer	-54.72	-54.72	-167.03	57.59	0.0910
Formamide dimer	-76.05	-76.05	-219.06	66.97	0.0610
Uracil dimer	-171.76	-171.76	-396.06	52.53	0.0440
Pyridoxine : aminopyridine	-68.61	-115.07	-222.77	39.09	0.2290
Adenine : thymine (WC)	-89.55	-201.01	-339.45	48.88	0.0470
Methane dimer	0.00	0.00	-2.53	2.53	0.0020
Ethene dimer	13.58	13.58	22.89	4.26	0.0620
Benzene : methane	12.60	0.00	7.91	4.69	0.0860
Benzene dimer (PD)	12.60	12.60	16.38	8.82	0.4300
Pyrazine dimer	90.01	90.01	157.21	22.81	0.3300

Uracil dimer	-171.76	-171.76	-374.08	30.55	0.1960
Indole : benzene (stacked)	12.60	-4.92	-6.83	14.51	0.8780
Adenine : thymine (stacked)	-89.55	-201.01	-331.49	40.93	0.3250
Ethene : ethyne	13.58	7.46	17.03	4.00	0.0970
Bezene : water	12.60	0.00	-3.54	16.14	0.1420
Benzene : ammonia	12.60	0.00	1.85	10.75	0.1370
Benzene : HCN	12.60	0.00	-3.23	15.83	0.1830
Benzene dimer (t-shaped)	12.60	12.60	16.32	8.87	2.3910
Indole : benzene (t-shaped)	12.60	-4.92	-17.91	25.59	0.0790
Phenol dimer	-12.39	-12.39	-62.55	37.77	0.5320

OPLSAA

Complex	Monomer A (kJ/mol)	Monomer B (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	RMS geometry (Å)
Ammonia dimer	0.00	0.00	-10.34	10.34	0.0330
Water dimer	0.00	0.00	-28.10	28.10	0.1240
Formic acid dimer	-59.29	-59.29	-171.34	52.75	0.1090
Formamide dimer	-95.49	-95.49	-248.73	57.75	0.0520
Uracil dimer	-146.10	-146.10	-345.21	53.01	0.0590
Pyridoxine : aminopyridine	0.87	-236.68	-277.29	41.48	0.2300
Adenine : thymine (WC)	-75.96	-168.26	-293.38	49.16	0.0450
Methane dimer	0.71	0.71	-0.78	2.19	0.0740
Ethene dimer	13.60	13.60	22.71	4.48	0.0520
Benzene : methane	27.95	0.71	24.21	4.45	0.0640
Benzene dimer (PD)	27.95	27.95	47.12	8.79	0.4300
Pyrazine dimer	110.54	110.54	198.33	22.74	0.3310
Uracil dimer	-146.10	-146.10	-322.26	30.05	0.2110
Indole : benzene (stacked)	27.95	10.09	13.27	24.78	1.2880
Adenine : thymine (stacked)	-75.96	-168.26	-285.48	41.25	0.3360
Ethene : ethyne	13.60	8.23	18.29	3.54	1.1160
Bezene : water	27.95	0.00	12.23	15.72	0.1330
Benzene : ammonia	27.95	0.00	18.91	9.05	0.0810
Benzene : HCN	27.95	0.00	12.88	15.08	0.1450
Benzene dimer (t-shaped)	27.95	27.95	47.05	8.86	0.1030
Indole : benzene (t-shaped)	27.95	10.09	13.50	24.54	0.0850
Phenol dimer	3.82	3.82	-25.57	33.22	0.3350

MMFF94

Complex	Monomer A (kJ/mol)	Monomer B (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	RMS geometry (Å)
Ammonia dimer	0.00	0.00	-12.65	12.65	0.0420
Water dimer	0.00	0.00	-27.65	27.65	0.1400
Formic acid dimer	-107.01	-107.01	-285.09	71.08	0.1420
Formamide dimer	-129.32	-129.32	-309.95	51.31	0.0430
Uracil dimer	-403.79	-403.79	-865.48	57.90	0.0800
Pyridoxine : aminopyridine	-24.42	-146.74	-214.04	42.88	0.0890
Adenine : thymine (WC)	-21.25	-396.10	-466.90	49.55	0.2110
Methane dimer	0.11	0.11	-1.44	1.66	0.0060
Ethene dimer	34.31	34.31	65.51	3.11	0.2420
Benzene : methane	67.89	0.11	65.41	2.60	0.2100
Benzene dimer (PD)	67.89	67.89	127.91	7.88	0.7230
Pyrazine dimer	219.82	219.82	419.32	20.32	0.3390
Uracil dimer	-403.79	-403.79	-858.61	51.03	2.0010
Indole : benzene (stacked)	67.89	63.23	110.09	21.03	1.3760
Adenine : thymine (stacked)	-21.25	-396.10	-470.61	53.26	1.9620
Ethene : ethyne	34.31	9.59	41.36	2.55	1.1320
Bezene : water	67.89	0.00	51.96	15.94	0.1220
Benzene : ammonia	67.89	0.00	57.54	10.36	0.1240
Benzene : HCN	67.89	0.00	52.57	15.32	0.2810
Benzene dimer (t-shaped)	67.89	67.89	128.35	7.44	0.2660
Indole : benzene (t-shaped)	67.89	63.23	110.19	20.93	0.1400
Phenol dimer	23.90	23.90	17.69	30.12	0.5240

MMFF94s

Complex	Monomer A (kJ/mol)	Monomer B (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	RMS geometry (Å)
Ammonia dimer	0.00	0.00	-12.65	12.65	0.0420
Water dimer	0.00	0.00	-27.65	27.65	0.1400
Formic acid dimer	-107.01	-107.01	-285.09	71.08	0.1420
Formamide dimer	-129.86	-129.86	-311.04	51.31	0.0430
Uracil dimer	-406.12	-406.12	-870.14	57.90	0.0800
Pyridoxine : aminopyridine	-25.46	-132.73	-202.54	44.34	0.1280
Adenine : thymine (WC)	-18.30	-398.43	-467.47	50.73	0.0560
Methane dimer	0.11	0.11	-1.44	1.66	0.0060
Ethene dimer	34.31	34.31	65.51	3.11	0.2420
Benzene : methane	67.89	0.11	65.41	2.60	0.2100
Benzene dimer (PD)	67.89	67.89	127.91	7.88	0.7230
Pyrazine dimer	219.82	219.82	419.32	20.32	0.3390

Uracil dimer	-406.12	-406.12	-863.27	51.03	2.0010
Indole : benzene (stacked)	67.89	63.23	110.09	21.03	1.3760
Adenine : thymine (stacked)	-18.30	-398.43	-470.05	53.31	2.0910
Ethene : ethyne	34.31	9.59	41.36	2.55	1.1320
Bezene : water	67.89	0.00	51.96	15.94	0.1220
Benzene : ammonia	67.89	0.00	57.54	10.36	0.1240
Benzene : HCN	67.89	0.00	52.57	15.32	0.2810
Benzene dimer (t-shaped)	67.89	67.89	128.35	7.44	0.2660
Indole : benzene (t-shaped)	67.89	63.23	110.19	20.93	0.1400
Phenol dimer	23.90	23.90	17.69	30.12	0.5240

S22 data set: Results with default bond dipole cut-offs (BDCOs)

MM2*

Complex	Monomer A (kJ/mol)	Monomer B (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	RMS geometry (Å)
Ammonia dimer	0.00	0.00	-3.00	3.00	0.1760
Water dimer	0.00	0.00	-13.35	13.35	0.2610
Formic acid dimer	-125.24	-125.24	-304.67	54.20	0.1880
Formamide dimer	-118.17	-118.17	-276.62	40.29	0.0900
Uracil dimer	-346.99	-346.99	-739.16	45.17	0.2160
Pyridoxine : aminopyridine	-103.50	-139.82	-257.13	13.82	0.4260
Adenine : thymine (WC)	95.54	-366.16	-289.42	18.80	1.5280
Methane dimer	0.00	0.00	-3.82	3.82	0.1100
Ethene dimer	1.77	1.77	-0.57	4.10	0.1500
Benzene : methane	12.56	0.00	7.53	5.03	0.0610
Benzene dimer (PD)	12.56	12.56	9.70	15.42	0.5480
Pyrazine dimer	197.66	197.66	373.50	21.83	0.3980
Uracil dimer	-346.99	-346.99	-735.14	41.16	2.3950
Indole : benzene (stacked)	12.56	60.12	53.54	19.14	0.3710
Adenine : thymine (stacked)	95.54	-366.16	-294.51	23.90	0.6750
Ethene : ethyne	1.77	-0.21	-0.43	1.99	0.1170
Bezene : water	12.56	0.00	7.90	4.66	0.2140
Benzene : ammonia	12.56	0.00	6.53	6.03	0.3770
Benzene : HCN	12.56	0.00	7.34	5.22	0.5100
Benzene dimer (t-shaped)	12.56	12.56	18.55	6.57	0.1340
Indole : benzene (t-shaped)	12.56	60.12	63.95	8.73	0.2140
Phenol dimer	15.47	15.47	14.11	16.83	2.1500

MM2* with explicit lone pairs

Complex	Monomer A (kJ/mol)	Monomer B (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	
Ammonia dimer	2.80	2.80	-1.26	6.87	0.4980
Water dimer	0.76	0.76	-18.87	20.39	0.1870
Formic acid dimer	30.15	30.15	0.86	59.44	0.1610
Formamide dimer	-118.17	-118.17	-276.62	40.29	0.1160
Uracil dimer	-346.99	-346.99	-739.16	45.17	0.1370
Pyridoxine : aminopyridine	-103.50	-139.82	-257.13	13.82	0.2840
Adenine : thymine (WC)	95.54	-366.16	-286.55	15.93	0.6760
Methane dimer	0.00	0.00	-3.82	3.82	0.1090
Ethene dimer	1.77	1.77	-0.57	4.10	0.1490
Benzene : methane	12.56	0.00	7.53	5.03	0.0490
Benzene dimer (PD)	12.56	12.56	9.70	15.42	0.4590
Pyrazine dimer	197.66	197.66	373.50	21.83	0.3460
Uracil dimer	-346.99	-346.99	-735.14	41.16	2.0450
Indole : benzene (stacked)	12.56	60.12	53.54	19.14	0.3120
Adenine : thymine (stacked)	95.54	-366.16	-294.51	23.90	0.6380
Ethene : ethyne	1.77	-0.21	-0.43	1.99	0.0230
Bezene : water	12.56	0.76	7.69	5.63	0.1290
Benzene : ammonia	12.56	2.80	9.04	6.32	0.1390
Benzene : HCN	12.56	0.00	7.34	5.22	0.4440
Benzene dimer (t-shaped)	12.56	12.56	18.55	6.57	2.3920
Indole : benzene (t-shaped)	12.56	60.12	63.95	8.73	0.2500
Phenol dimer	16.02	16.02	12.50	19.53	1.7270

MM3*

Complex	Monomer A (kJ/mol)	Monomer B (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	
Ammonia dimer	0.00	0.00	-4.86	4.86	0.2130
Water dimer	0.00	0.00	-29.75	29.75	0.3220
Formic acid dimer	-26.85	-26.85	-70.22	16.52	0.1900
Formamide dimer	-54.64	-54.64	-144.78	35.50	0.0820
Uracil dimer	-705.99	-705.99	-1429.33	17.35	0.1550
Pyridoxine : aminopyridine	-61.18	-170.89	-247.14	15.06	0.8800
Adenine : thymine (WC)	-243.05	-707.54	-965.62	15.03	0.5240
Methane dimer	0.00	0.00	-1.73	1.73	0.0270
Ethene dimer	29.32	29.32	55.42	3.21	0.2040
Benzene : methane	25.55	0.00	21.96	3.59	0.1300

Benzene dimer (PD)	25.55	25.55	41.03	10.08	0.2590
Pyrazine dimer	135.46	135.46	250.84	20.07	0.3900
Uracil dimer	-705.99	-705.99	-1427.43	15.45	0.2940
Indole : benzene (stacked)	25.55	107.05	117.13	15.48	0.4600
Adenine : thymine (stacked)	-242.69	-707.54	-982.24	32.01	0.6110
Ethene : ethyne	29.32	13.55	40.13	2.73	0.0970
Bezene : water	25.55	0.00	14.53	11.03	0.2090
Benzene : ammonia	25.55	0.00	17.68	7.87	0.3490
Benzene : HCN	25.55	0.00	12.71	12.84	0.3410
Benzene dimer (t-shaped)	25.55	25.55	43.44	7.66	0.1390
Indole : benzene (t-shaped)	25.55	107.05	123.41	9.20	1.0010
Phenol dimer	10.30	10.30	7.68	12.93	1.0660

AMBER*

Complex	**Monomer A (kJ/mol)**	**Monomer B (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	
Ammonia dimer	0.00	0.00	-19.43	19.43	0.1930
Water dimer	0.00	0.00	-29.92	29.92	0.1940
Formic acid dimer	-46.69	-46.69	-136.79	43.41	0.1760
Formamide dimer	-83.24	-83.24	-226.60	60.13	0.0500
Uracil dimer	-336.61	-336.61	-715.44	42.23	0.1120
Pyridoxine : aminopyridine	-115.65	-74.66	-240.41	50.10	0.5220
Adenine : thymine (WC)	-363.58	-631.08	-1040.67	46.01	0.1680
Methane dimer	0.00	0.00	-1.29	1.29	0.0810
Ethene dimer	23.46	23.46	42.83	4.09	0.0800
Benzene : methane	29.10	0.00	25.55	3.56	0.0770
Benzene dimer (PD)	29.10	29.10	46.31	11.90	0.5520
Pyrazine dimer	106.95	106.95	186.29	27.61	0.3940
Uracil dimer	-336.61	-336.61	-709.33	36.12	0.2490
Indole : benzene (stacked)	29.10	5.13	7.65	26.59	1.5560
Adenine : thymine (stacked)	-364.61	-631.08	-1040.27	44.59	0.4280
Ethene : ethyne	23.46	18.80	37.94	4.32	0.0230
Bezene : water	29.10	0.00	5.94	23.17	0.2150
Benzene : ammonia	29.10	0.00	14.71	14.39	0.1980
Benzene : HCN	29.10	0.00	4.38	24.73	0.2990
Benzene dimer (t-shaped)	29.10	29.10	47.31	10.89	0.0780
Indole : benzene (t-shaped)	29.10	5.13	7.91	26.33	0.0860
Phenol dimer	4.02	4.02	-20.73	28.78	0.4290

AMBER* (10,12 H-bonding potential)

Complex	**Monomer A (kJ/mol)**	**Monomer B (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	
Ammonia dimer	0.00	0.00	-19.43	19.43	0.1600
Water dimer	0.00	0.00	-29.92	29.92	0.1220
Formic acid dimer	-46.69	-46.69	-136.79	43.41	0.1610
Formamide dimer	-83.24	-83.24	-226.60	60.13	0.0470
Uracil dimer	-336.61	-336.61	-715.44	42.23	0.0920
Pyridoxine : aminopyridine	-115.65	-74.66	-240.41	50.10	0.4250
Adenine : thymine (WC)	-363.58	-631.08	-1040.67	46.01	0.0720
Methane dimer	0.00	0.00	-1.29	1.29	0.0820
Ethene dimer	23.46	23.46	42.83	4.09	0.0790
Benzene : methane	29.10	0.00	25.55	3.56	0.0640
Benzene dimer (PD)	29.10	29.10	46.31	11.90	0.5030
Pyrazine dimer	106.95	106.95	186.29	27.61	0.3380
Uracil dimer	-336.61	-336.61	-709.33	36.12	0.2300
Indole : benzene (stacked)	29.10	5.13	7.65	26.59	1.2840
Adenine : thymine (stacked)	-364.61	-631.08	-1040.27	44.59	0.3300
Ethene : ethyne	23.46	18.80	37.94	4.32	0.0190
Bezene : water	29.10	0.00	5.94	23.17	0.1910
Benzene : ammonia	29.10	0.00	14.71	14.39	0.1650
Benzene : HCN	29.10	0.00	4.38	24.73	0.2760
Benzene dimer (t-shaped)	29.10	29.10	47.31	10.89	0.0780
Indole : benzene (t-shaped)	29.10	5.13	7.91	26.33	0.0840
Phenol dimer	4.02	4.02	-20.73	28.78	0.3490

OPLS*

Complex	**Monomer A (kJ/mol)**	**Monomer B (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	
Ammonia dimer	0.00	0.00	-17.05	17.05	0.1870
Water dimer	0.00	0.00	-28.61	28.61	0.1930
Formic acid dimer	-54.72	-54.72	-167.03	57.59	0.1010
Formamide dimer	-76.05	-76.05	-219.06	66.97	0.0880
Uracil dimer	-171.76	-171.76	-395.51	51.99	0.0580
Pyridoxine : aminopyridine	-68.61	-115.07	-222.77	39.09	0.2500
Adenine : thymine (WC)	-89.55	-201.01	-334.62	44.05	0.0540
Methane dimer	0.00	0.00	-2.53	2.53	0.0020
Ethene dimer	13.58	13.58	22.89	4.26	0.0640
Benzene : methane	12.60	0.00	7.91	4.69	0.1040

Benzene dimer (PD)	12.60	12.60	16.38	8.82	0.4590
Pyrazine dimer	90.01	90.01	157.21	22.81	0.3880
Uracil dimer	-171.76	-171.76	-374.08	30.55	0.2140
Indole : benzene (stacked)	12.60	-4.92	-6.83	14.51	1.0400
Adenine : thymine (stacked)	-89.55	-201.01	-331.49	40.93	0.3220
Ethene : ethyne	13.58	7.46	17.03	4.00	0.0970
Bezene : water	12.60	0.00	-3.54	16.14	0.1490
Benzene : ammonia	12.60	0.00	1.85	10.75	0.1840
Benzene : HCN	12.60	0.00	-3.23	15.83	0.1970
Benzene dimer (t-shaped)	12.60	12.60	16.33	8.87	0.1000
Indole : benzene (t-shaped)	12.60	-4.92	-17.91	25.59	0.0790
Phenol dimer	-12.39	-12.39	-62.55	37.76	0.6260

OPLSAA

Complex	Monomer A (kJ/mol)	Monomer B (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	
Ammonia dimer	0.00	0.00	-10.34	10.34	0.0670
Water dimer	0.00	0.00	-28.10	28.10	0.1610
Formic acid dimer	-59.29	-59.29	-171.34	52.75	0.1180
Formamide dimer	-95.49	-95.49	-248.73	57.75	0.0430
Uracil dimer	-146.10	-146.10	-344.23	52.02	0.0740
Pyridoxine : aminopyridine	0.87	-236.68	-277.29	41.48	0.2540
Adenine : thymine (WC)	-75.96	-168.26	-288.35	44.13	0.0520
Methane dimer	0.71	0.71	-0.78	2.19	0.0740
Ethene dimer	13.60	13.60	22.71	4.48	0.0520
Benzene : methane	27.95	0.71	24.21	4.45	0.0760
Benzene dimer (PD)	27.95	27.95	47.11	8.79	0.4540
Pyrazine dimer	110.54	110.54	198.33	22.74	0.3890
Uracil dimer	-146.10	-146.10	-322.26	30.05	0.2040
Indole : benzene (stacked)	27.95	10.09	13.27	24.78	1.5620
Adenine : thymine (stacked)	-75.96	-168.26	-285.48	41.25	0.3840
Ethene : ethyne	13.60	8.23	18.29	3.54	0.0190
Bezene : water	27.95	0.00	12.23	15.72	0.1330
Benzene : ammonia	27.95	0.00	18.91	9.05	0.0970
Benzene : HCN	27.95	0.00	12.88	15.08	0.2520
Benzene dimer (t-shaped)	27.95	27.95	47.05	8.86	0.1030
Indole : benzene (t-shaped)	27.95	10.09	13.50	24.54	0.0880
Phenol dimer	3.82	3.82	-25.57	33.22	0.3990

MMFF94

Complex	Monomer A (kJ/mol)	Monomer B (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	
Ammonia dimer	0.00	0.00	-12.65	12.65	0.0560
Water dimer	0.00	0.00	-27.65	27.65	0.2090
Formic acid dimer	-107.01	-107.01	-285.09	71.08	0.1290
Formamide dimer	-129.32	-129.32	-309.95	51.31	0.0380
Uracil dimer	-403.79	-403.79	-865.48	57.90	0.0900
Pyridoxine : aminopyridine	-24.42	-146.74	-214.04	42.88	0.1430
Adenine : thymine (WC)	-21.25	-396.10	-465.02	47.67	0.2350
Methane dimer	0.11	0.11	-1.44	1.66	0.0070
Ethene dimer	34.31	34.31	65.51	3.11	0.2420
Benzene : methane	67.89	0.11	65.41	2.60	0.2560
Benzene dimer (PD)	67.89	67.89	127.91	7.88	0.7630
Pyrazine dimer	219.82	219.82	419.32	20.32	0.3960
Uracil dimer	-403.79	-403.79	-858.61	51.03	2.3410
Indole : benzene (stacked)	67.89	63.23	110.09	21.03	1.6340
Adenine : thymine (stacked)	-21.25	-396.10	-470.48	53.13	2.2980
Ethene : ethyne	34.31	9.59	41.36	2.55	0.2070
Bezene : water	67.89	0.00	51.96	15.94	0.2130
Benzene : ammonia	67.89	0.00	57.54	10.36	0.1910
Benzene : HCN	67.89	0.00	52.57	15.32	0.3190
Benzene dimer (t-shaped)	67.89	67.89	128.35	7.44	0.2660
Indole : benzene (t-shaped)	67.89	63.23	110.19	20.93	0.1440
Phenol dimer	23.90	23.90	17.69	30.12	0.6180

MMFF94s

Complex	Monomer A (kJ/mol)	Monomer B (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	
Ammonia dimer	0.00	0.00	-12.65	12.65	0.0560
Water dimer	0.00	0.00	-27.65	27.65	0.2090
Formic acid dimer	-107.01	-107.01	-285.09	71.08	0.1290
Formamide dimer	-129.86	-129.86	-311.04	51.31	0.0380
Uracil dimer	-406.12	-406.12	-870.14	57.90	0.0900
Pyridoxine : aminopyridine	-25.46	-132.73	-202.54	44.34	0.1570
Adenine : thymine (WC)	-18.30	-398.43	-465.20	48.47	0.0580
Methane dimer	0.11	0.11	-1.44	1.66	0.0070
Ethene dimer	34.31	34.31	65.51	3.11	0.2420
Benzene : methane	67.89	0.11	65.41	2.60	0.2560

Benzene dimer (PD)	67.89	67.89	127.91	7.88	0.7630
Pyrazine dimer	219.82	219.82	419.32	20.32	0.3960
Uracil dimer	-406.12	-406.12	-863.27	51.03	2.3410
Indole : benzene (stacked)	67.89	63.23	110.09	21.03	1.6340
Adenine : thymine (stacked)	-18.30	-398.43	-469.73	53.00	2.4510
Ethene : ethyne	34.31	9.59	41.36	2.55	0.2070
Bezene : water	67.89	0.00	51.96	15.94	0.2130
Benzene : ammonia	67.89	0.00	57.54	10.36	0.1910
Benzene : HCN	67.89	0.00	52.57	15.32	0.3190
Benzene dimer (t-shaped)	67.89	67.89	128.35	7.44	0.2660
Indole : benzene (t-shaped)	67.89	63.23	110.19	20.93	0.1440
Phenol dimer	23.90	23.90	17.69	30.12	0.6180