Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting material of logarithmic activity coefficient of three cellulose models-revised

logarithmic activity coefficient of glucose model

	Empyrr	EtOMmpyrr	Eemor	Ampyrr	Aemor	EtOMemor	Amim	Emim	EtOMmim	Epy	EtOMpy	Apy	AOPmim	HOEtmpyrr	HOEtmim	HOEtemor	HOEtpy
Ac	-2.87	-2.81	-2.66	-2.66	-2.58	-2.53	-2.47	-2.44	-2.42	-2.41	-2.39	-2.38	-2.38	-2.20	-1.89	-1.83	-1.78
Dec	-2.67	-2.62	-2.54	-2.50	-2.46	-2.42	-2.35	-2.32	-2.30	-2.32	-2.30	-2.30	-2.28	-2.09	-1.87	-1.88	-1.80
HCOO	-2.52	-2.47	-2.31	-2.32	-2.23	-2.19	-2.15	-2.12	-2.11	-2.08	-2.06	-2.05	-2.07	-1.92	-1.62	-1.53	-1.50
Cl	-2.36	-2.29	-2.12	-2.13	-2.04	-1.98	-1.98	-1.96	-1.93	-1.90	-1.87	-1.86	-1.88	-1.84	-1.51	-1.38	-1.39
DEP	-2.27	-2.22	-2.11	-2.11	-2.05	-2.01	-1.98	-1.97	-1.95	-1.94	-1.92	-1.92	-1.91	-1.82	-1.59	-1.52	-1.51
DMPO4	-2.24	-2.19	-2.06	-2.07	-1.99	-1.95	-1.93	-1.92	-1.90	-1.88	-1.86	-1.86	-1.86	-1.77	-1.52	-1.44	-1.43
DBP	-2.20	-2.15	-2.07	-2.06	-2.01	-1.97	-1.95	-1.94	-1.91	-1.92	-1.89	-1.89	-1.88	-1.79	-1.60	-1.56	-1.53
BEN	-2.14	-2.10	-1.99	-1.99	-1.93	-1.90	-1.83	-1.82	-1.81	-1.79	-1.78	-1.76	-1.78	-1.63	-1.40	-1.38	-1.31
Br	-1.70	-1.65	-1.49	-1.52	-1.42	-1.38	-1.37	-1.37	-1.35	-1.29	-1.28	-1.26	-1.30	-1.30	-1.01	-0.89	-0.89
Tos	-1.50	-1.47	-1.37	-1.38	-1.32	-1.30	-1.27	-1.28	-1.26	-1.24	-1.23	-0.10	-1.23	-1.21	-1.03	-0.96	-0.96
$MeOEtSO_4$	-1.14	-1.12	-1.03	-1.04	-0.99	-0.96	-0.97	-0.98	-0.96	-0.94	-0.93	-0.92	-0.93	-0.92	-0.77	-0.68	-0.71
$BuSO_4$	-1.14	-1.11	-1.03	-1.04	-0.99	-0.97	-0.97	-0.98	-0.96	-0.95	-0.93	-0.93	-0.94	-0.93	-0.79	-0.72	-0.74
$MeSO_4$	-1.08	-1.06	-0.95	-0.97	-0.91	-0.89	-0.89	-0.90	-0.89	-0.85	-0.84	-0.83	-0.86	-0.83	-0.66	-0.56	-0.59
I	-1.05	-1.02	-0.88	-0.92	-0.84	-0.81	-0.81	-0.81	-0.80	-0.74	-0.74	-0.71	-0.77	-0.77	-0.55	-0.43	-0.45
$N(CN)_2$	-0.97	-0.96	-0.85	-0.88	-0.82	-0.81	-0.75	-0.76	-0.76	-0.70	-0.70	-0.67	-0.73	-0.72	-0.54	-0.49	-0.45
HSO_4	-0.85	-0.85	-0.72	-0.76	-0.70	-0.68	-0.68	-0.67	-0.68	-0.62	-0.63	-0.61	-0.68	-0.60	-0.42	-0.32	-0.34
BF_4	-0.49	-0.49	-0.39	-0.44	-0.38	-0.36	-0.38	-0.38	-0.39	-0.34	-0.35	-0.33	-0.38	-0.35	-0.23	-0.13	-0.17
ClO_4	-0.31	-0.32	-0.23	-0.27	-0.22	-0.21	-0.23	-0.23	-0.23	-0.19	-0.20	-0.19	-0.23	-0.21	-0.12	-0.02	-0.07
$AlCl_4$	-0.10	-0.08	-0.08	-0.11	-0.08	-0.07	-0.10	-0.13	-0.11	-0.12	-0.10	-0.10	-0.06	-0.17	-0.20	-0.16	-0.21
PF_6	-0.16	-0.16	-0.10	-0.15	-0.11	-0.10	-0.12	-0.14	-0.14	-0.11	-0.11	-0.10	-0.11	-0.15	-0.11	-0.04	-0.09
Tf_2N	-0.21	-0.19	-0.19	-0.19	-0.17	-0.17	-0.16	-0.19	-0.18	-0.18	-0.16	-0.15	-0.14	-0.23	-0.22	-0.20	-0.21

logarithmic activity coefficient of mid-monomer part of a cellotriose model

	Empyrr	EtOMmpyrr	Eemor	Ampyrr	Aemor	EtOMemor	Amim	Emim	Epy	EtOMmim	EtOMpy	Apy	AOPmim	HOEtmpyrr	HOEtmim	HOEtemor	HOEtpy
Ac	-2.02	-1.93	-1.82	-1.81	-1.73	-1.69	-1.65	-1.65	-1.62	-1.61	-1.58	-1.57	-1.52	-1.51	-1.24	-1.18	-1.15
Dec	-1.75	-1.69	-1.62	-1.60	-1.55	-1.52	-1.48	-1.46	-1.46	-1.43	-1.43	-1.43	-1.39	-1.33	-1.14	-1.15	-1.09
HCOO	-1.73	-1.64	-1.53	-1.52	-1.44	-1.40	-1.38	-1.39	-1.35	-1.34	-1.31	-1.30	-1.26	-1.28	-1.02	-0.95	-0.93
Cl	-1.51	-1.40	-1.31	-1.30	-1.21	-1.16	-1.17	-1.20	-1.15	-1.13	-1.09	-1.08	-1.03	-1.15	-0.90	-0.79	-0.80
BEN	-1.49	-1.43	-1.35	-1.34	-1.28	-1.26	-1.20	-1.20	-1.18	-1.18	-1.16	-1.14	-1.11	-1.09	-0.89	-0.88	-0.82
DMPO4	-1.35	-1.28	-1.20	-1.20	-1.14	-1.10	-1.09	-1.10	-1.07	-1.07	-1.04	-1.03	-1.00	-1.03	-0.84	-0.78	-0.77
DEP	-1.33	-1.27	-1.20	-1.20	-1.14	-1.11	-1.10	-1.10	-1.08	-1.07	-1.05	-1.05	-1.02	-1.03	-0.86	-0.82	-0.80
DBP	-1.22	-1.17	-1.12	-1.11	-1.07	-1.05	-1.03	-1.03	-1.02	-1.00	-0.99	-0.99	-0.96	-0.96	-0.82	-0.81	-0.78
Br	-1.05	-0.97	-0.87	-0.88	-0.80	-0.76	-0.75	-0.78	-0.72	-0.73	-0.68	-0.66	-0.65	-0.78	-0.55	-0.46	-0.46
Tos	-0.77	-0.73	-0.67	-0.68	-0.63	-0.62	-0.59	-0.61	-0.59	-0.59	-0.57	-0.55	-0.54	-0.60	-0.48	-0.45	-0.43
I	-0.64	-0.58	-0.50	-0.51	-0.44	-0.42	-0.41	-0.44	-0.39	-0.41	-0.36	-0.34	-0.35	-0.46	-0.29	-0.20	-0.20
$MeSO_4$	-0.58	-0.54	-0.48	-0.49	-0.44	-0.42	-0.42	-0.45	-0.41	-0.42	-0.39	-0.38	-0.37	-0.44	-0.32	-0.25	-0.26
$MeOEtSO_4$	-0.57	-0.53	-0.49	-0.50	-0.45	-0.44	-0.44	-0.46	-0.44	-0.44	-0.41	-0.40	-0.39	-0.46	-0.36	-0.31	-0.32
$BuSO_4$	-0.55	-0.52	-0.48	-0.49	-0.45	-0.43	-0.43	-0.46	-0.44	-0.43	-0.41	-0.40	-0.39	-0.45	-0.37	-0.33	-0.34
$N(CN)_2$	-0.55	-0.52	-0.44	-0.47	-0.41	-0.41	-0.35	-0.38	-0.33	-0.37	-0.32	-0.29	-0.32	-0.40	-0.25	-0.23	-0.19
HSO_4	-0.49	-0.46	-0.38	-0.40	-0.35	-0.34	-0.33	-0.34	-0.30	-0.34	-0.30	-0.28	-0.31	-0.33	-0.19	-0.12	-0.13
BF_4	-0.28	-0.26	-0.20	-0.23	-0.18	-0.18	-0.19	-0.21	-0.17	-0.20	-0.17	-0.15	-0.16	-0.23	-0.14	-0.06	-0.10
ClO_4	-0.19	-0.18	-0.13	-0.16	-0.12	-0.11	-0.12	-0.15	-0.11	-0.14	-0.11	-0.10	-0.10	-0.18	-0.11	-0.04	-0.09
PF_6	-0.14	-0.13	-0.10	-0.14	-0.11	-0.10	-0.12	-0.15	-0.13	-0.14	-0.13	-0.11	-0.10	-0.21	-0.21	-0.16	-0.20
$AlCl_4$	-0.12	-0.10	-0.13	-0.16	-0.14	-0.14	-0.16	-0.21	-0.21	-0.18	-0.18	-0.18	-0.11	-0.29	-0.36	-0.35	-0.39
Tf_2N	-0.07	-0.05	-0.08	-0.07	-0.07	-0.07	-0.06	-0.10	-0.10	-0.08	-0.08	-0.07	-0.03	-0.18	-0.21	-0.22	-0.23

logarithmic activity coefficient of mid-dimer part of the cellotetraose model

	Empyrr	EtOMmpyrr	Eemor	Ampyrr	AOPmim	Aemor	EtOMmim	EtOMemor	Amim	Emim	Epy	EtOMpy	Apy	HOEtmpyrr	HOEtmim	HOEtemor	HOEtPy
Ac	-2.16	-2.10	-1.99	-1.98	-1.95	-1.91	-1.90	-1.87	-1.84	-1.82	-1.80	-1.77	-1.77	-1.63	-1.38	-1.33	-1.29
Dec	-1.88	-1.82	-1.78	-1.75	-1.68	-1.71	-1.73	-1.68	-1.63	-1.62	-1.63	-1.59	-1.59	-1.44	-1.28	-1.29	-1.23
HCOO	-1.83	-1.77	-1.66	-1.66	-1.66	-1.58	-1.72	-1.55	-1.52	-1.52	-1.49	-1.46	-1.45	-1.36	-1.12	-1.05	-1.04
Cl	-1.59	-1.52	-1.41	-1.41	-1.49	-1.33	-1.55	-1.29	-1.29	-1.29	-1.25	-1.21	-1.20	-1.21	-0.95	-0.85	-0.86
BEN	-1.53	-1.48	-1.41	-1.40	-1.34	-1.35	-1.40	-1.33	-1.28	-1.28	-1.27	-1.24	-1.23	-1.14	-0.97	-0.96	-0.90
DEP	-1.48	-1.42	-1.36	-1.35	-1.39	-1.30	-1.45	-1.27	-1.25	-1.25	-1.24	-1.20	-1.20	-1.15	-0.98	-0.93	-0.92
DMPO4	-1.48	-1.43	-1.34	-1.34	-1.39	-1.28	-1.45	-1.25	-1.24	-1.24	-1.22	-1.19	-1.18	-1.14	-0.95	-0.89	-0.88
DBP	-1.36	-1.31	-1.27	-1.25	-1.27	-1.21	-1.33	-1.19	-1.16	-1.17	-1.16	-1.13	-1.13	-1.07	-0.94	-0.92	-0.89
Br	-1.07	-1.02	-0.91	-0.93	-0.97	-0.85	-1.03	-0.82	-0.81	-0.82	-0.76	-0.74	-0.72	-0.79	-0.57	-0.47	-0.48
Tos	-0.85	-0.81	-0.75	-0.75	-0.79	-0.70	-0.85	-0.18	-0.67	-0.69	-0.66	-0.64	-0.63	-0.67	-0.53	-0.49	-0.49
$MeOEtSO_4$	-0.63	-0.60	-0.54	-0.55	-0.58	-0.50	-0.63	-0.48	-0.49	-0.52	-0.49	-0.46	-0.46	-0.50	-0.39	-0.33	-0.35
$BuSO_4$	-0.62	-0.58	-0.54	-0.54	-0.56	-0.50	-0.61	-0.48	-0.49	-0.51	-0.49	-0.47	-0.46	-0.50	-0.41	-0.36	-0.38
$MeSO_4$	-0.62	-0.59	-0.51	-0.53	-0.56	-0.48	-0.61	-0.46	-0.47	-0.49	-0.46	-0.44	-0.43	-0.47	-0.34	-0.26	-0.30
I	-0.64	-0.61	-0.50	-0.54	-0.54	-0.47	-0.60	-0.44	-0.45	-0.46	-0.41	-0.39	-0.37	-0.46	-0.29	-0.19	-0.22
$N(CN)_2$	-0.58	-0.56	-0.48	-0.51	-0.48	-0.45	-0.54	-0.44	-0.40	-0.43	-0.38	-0.37	-0.35	-0.43	-0.29	-0.26	-0.24
HSO_4	-0.50	-0.49	-0.39	-0.42	-0.47	-0.37	-0.50	-0.36	-0.36	-0.37	-0.33	-0.33	-0.31	-0.34	-0.21	-0.13	-0.16
$AlCl_4$	-0.19	-0.16	-0.19	-0.21	-0.11	-0.19	-0.20	-0.18	-0.22	-0.26	-0.26	-0.23	-0.23	-0.32	-0.38	-0.37	-0.41
BF_4	-0.32	-0.31	-0.23	-0.28	-0.27	-0.22	-0.31	-0.21	-0.24	-0.26	-0.22	-0.21	-0.20	-0.26	-0.18	-0.10	-0.15
PF_6	-0.20	-0.19	-0.16	-0.20	-0.15	-0.16	-0.21	-0.15	-0.19	-0.22	-0.20	-0.19	-0.18	-0.25	-0.25	-0.20	-0.25
ClO_4	-0.23	-0.22	-0.16	-0.20	-0.17	-0.16	-0.22	-0.14	-0.17	-0.19	-0.16	-0.16	-0.15	-0.21	-0.15	-0.07	-0.13
Tf_2N	-0.12	-0.09	-0.11	-0.12	-0.02	-0.10	-0.10	-0.10	-0.10	-0.14	-0.14	-0.11	-0.11	-0.21	-0.23	-0.23	-0.25