Supporting Information for: Recent Advances in the Continuous Fractional Component Monte Carlo Methodology

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Table S1. Chemical potentials of water (TIP3P [1]) and hydrogen (Marx [2]) in the gas phase, from vapor-liquid equilibrium simulations of binary water-hydrogen mixtures in the CFCMC Gibbs ensemble. Simulation details on the phase coexistence of the water-hydrogen systems are provided in Ref. [3]. The chemical potentials divided by k_B are in units of [K]. σ is the uncertainty.

P/[bar]	T/[K]	$\mu_{H_2O}/[k_B]$	σ	$\mu_{H_2}/[k_B]$	σ
50	423	-3930	14	-3034	4
80	423	-3926	14	-2809	4
100	423	-3914	13	-2706	3
300	423	-3873	13	-2183	3
500	423	-3819	15	-1925	3
800	423	-3749	14	-1666	4
1000	423	-3711	22	-1534	4
10	366	-3976	20	-3165	4
50	366	-3964	22	-2536	3
80	366	-3958	20	-2355	3
100	366	-3953	17	-2269	4
300	366	-3899	44	-1827	3
500	366	-3855	58	-1602	3
800	366	-3793	90	-1371	3
1000	366	-3761	100	-1251	3
10	323	-4037	21	-2720	3
50	323	-4038	69	-2189	3
80	323	-4023	104	-2031	3
100	323	-3994	78	-1955	2
300	323	-3986	120	-1565	3
500	323	-3952	144	-1363	3
800	323	-3869	123	-1155	2
1000	323	-3771	120	-1046	3

Table S2. Chemical potentials of water (TIP3P [1]) and hydrogen (Marx [2]) in the liquid phase, from vapor-liquid equilibrium simulations of binary water-hydrogen mixtures in the CFCMC Gibbs ensemble. Simulation details on the phase coexistence of the water-hydrogen systems are provided in Ref. [3]. The chemical potentials divided by k_{B} are in units of [K]. σ is the uncertainty.

P/[bar]	T/[K]	$\mu_{\mathrm{H_2O}}/[k_B]$	σ	$\mu_{\mathrm{H_2}}/[k_B]$	σ
50	423	-3929	13	-3037	6
80	423	-3926	13	-2811	5
100	423	-3914	13	-2708	5
300	423	-3874	13	-2185	5
500	423	-3819	14	-1927	5
800	423	-3749	13	-1669	5
1000	423	-3710	24	-1536	5
10	366	-3976	21	-3167	8
50	366	-3963	22	-2537	8
80	366	-3958	19	-2355	11
100	366	-3953	17	-2273	7
300	366	-3899	47	-1829	10
500	366	-3855	61	-1600	12
800	366	-3788	92	-1378	13
1000	366	-3761	105	-1250	14
10	323	-4037	21	-2723	21
50	323	-4038	72	-2189	19
80	323	-4020	111	-2036	15
100	323	-3990	80	-1961	21
300	323	-3983	124	-1570	21
500	323	-3948	147	-1371	24
800	323	-3867	129	-1157	16
1000	323	-3772	123	-1045	21

References

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