Supporting Information for:

Title

Physical Properties and Characterization of the Binary Clathrate Hydrate with Methane + 1,1,1,3,3-pentafluoropropane (HFC-245fa) + Water

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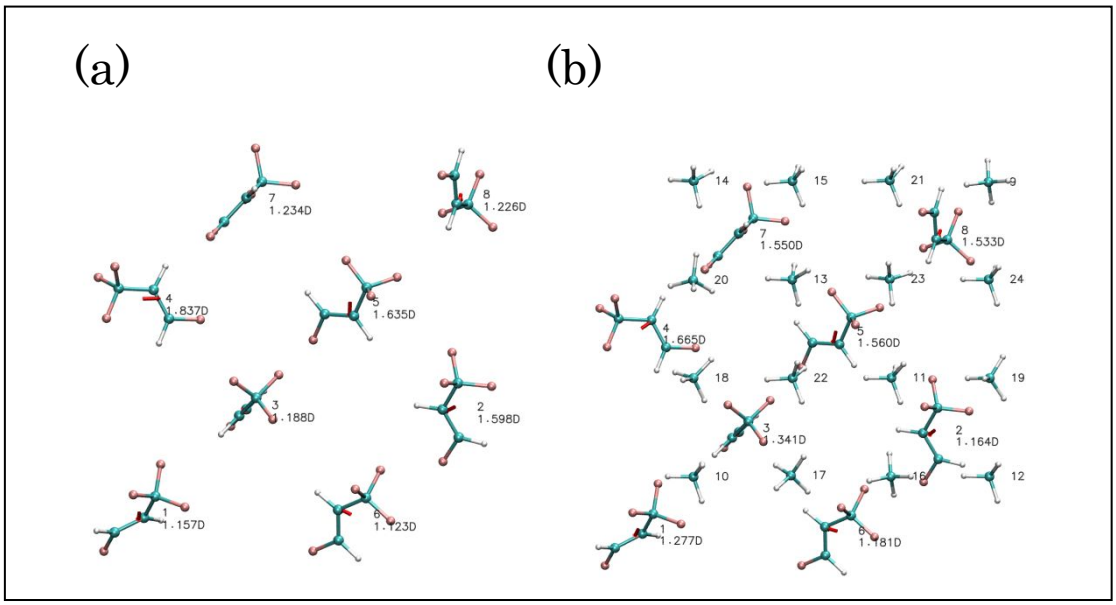

Figure S1. The value and vector of dipole moments and the positions of guest molecules in the optimized HFO-1234ze(E) hydrate (a) and HFO-1234ze(E) + CH_4 hydrate (b) structures, respectively.

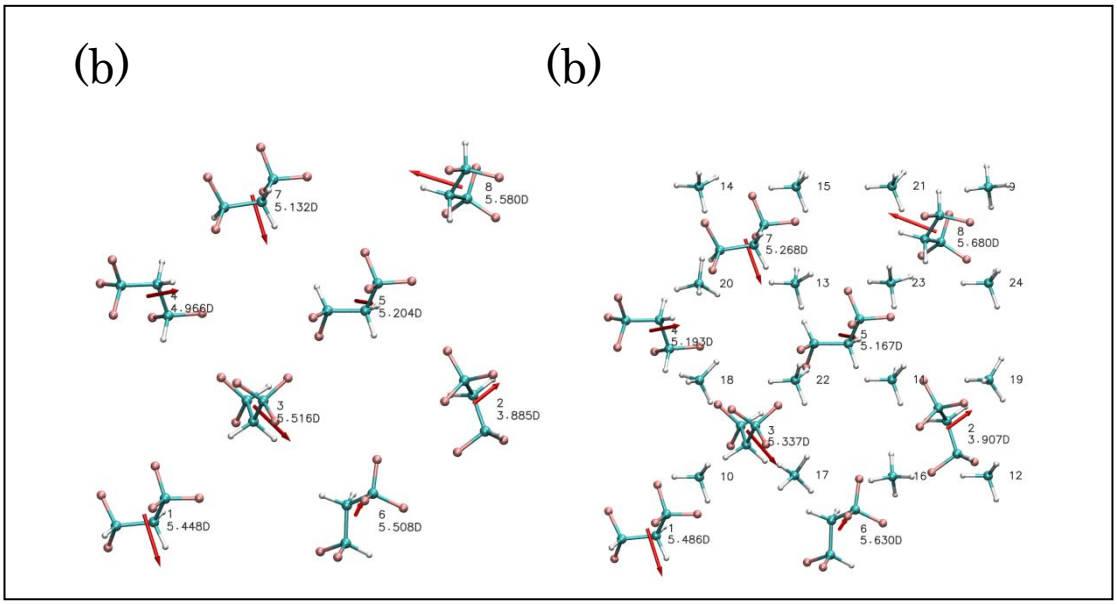

Figure S2. The value and vector of dipole moments and the positions of guest molecules in the optimized HFC-245fa hydrate (a) and HFC-245fa + CH_4 hydrate (b) structures, respectively.

Table S1. Bader Charge of HFO-1234ze(E) and HFC-245fa molecules (the atom number corresponds to atoms presented in Figure 1) in single and binary sII hydrates and gas phase.

System	HFO-1234ze(E) // HFO-1234ze(E) + CH_4 // HFO-1234ze(E) (mono)							
GUESTS	HFO-1234ze(E)							
	1	2	3	4	5	6	7	8
C_1	+1.623// +1.638// +1.630	+1.658// +1.659// +1.630	+1.629// +1.654// +1.630	+1.602// +1.593// +1.630	+1.652// +1.624// +1.630	+1.634// +1.621// +1.630	+1.641// +1.640// +1.630	+1.644/ +1.644// +1.630
F_1	-0.595// -0.617// -0.595	-0.605// -0.607// -0.595	-0.603// -0.605// -0.595	-0.605// -0.601// -0.595	-0.614// -0.598// -0.595	-0.597// -0.596// -0.595	-0.600// -0.599// -0.595	-0.604// -0.603// -0.595
F_2	-0.611// -0.611// -0.605	-0.638// -0.632// -0.605	-0.612// -0.624// -0.605	-0.615// -0.612// -0.605	-0.620// -0.613// -0.605	-0.605// -0.607// -0.605	-0.622// -0.623// -0.605	-0.610// -0.617// -0.605
F_3	-0.613// -0.614// -0.604	-0.610// -0.610// -0.604	-0.610// -0.615// -0.604	-0.609// -0.609// -0.604	-0.615// -0.611// -0.604	-0.602// -0.603// -0.604	-0.614// -0.614// -0.604	-0.610// -0.613// -0.604
C_2	+0.170// +0.158// +0.158	+0.096// +0.204// +0.158	+0.170// +0.144// +0.158	+0.077// +0.229// +0.158	+0.125// +0.116// +0.158	+0.221// +0.223// +0.158	+0.206// +0.130// +0.158	+0.212// +0.185// +0.158
H_1	+0.125// +0.129// +0.149	+0.216// +0.122// +0.149	+0.148// +0.168// +0.149	+0.185// +0.194// +0.149	+0.161// +0.149// +0.149	+0.148// +0.149// +0.149	+0.183// +0.191// +0.149	+0.135// +0.144// +0.149
C_3	+0.302// +0.297// +0.294	+0.291// +0.273// +0.294	+0.285// +0.314// +0.294	+0.377// +0.217// +0.294	+0.372// +0.392// +0.294	+0.215// +0.212// +0.294	+0.276// +0.291// +0.294	+0.254// +0.340// +0.294
F_5	-0.640// -0.638// -0.615	-0.634// -0.631// -0.615	-0.632// -0.636// -0.615	-0.629// -0.629// -0.615	-0.630// -0.628// -0.615	-0.632// -0.622// -0.615	-0.628// -0.627// -0.615	-0.623// -0.626// -0.615
H_2	+0.205// +0.223// +0.188	+0.194// +0.190// +0.188	+0.197// +0.171// +0.188	+0.188// +0.190// +0.188	+0.136// +0.137// +0.188	+0.187// +0.191// +0.188	+0.125// +0.179// +0.188	+0.176// +0.120// +0.188

System	HFC-245fa // HFC-245fa + CH_4 // HFC-245fa (mono)							
GUESTS	HFC-245fa							
	1	2	3	4	5	6	7	8
C_1	+1.686/ +1.681// +1.663	+1.649// +1.672// +1.663	+1.678// +1.667// +1.663	+1.706// +1.687// +1.663	+1.714// +1.694// +1.663	+1.621// +1.647// +1.663	+1.621// +1.599// +1.663	+1.666// +1.666// +1.663
F_1	-0.628// -0.637// -0.600	-0.614// -0.619// -0.600	-0.615// -0.613// -0.600	-0.612// -0.609// -0.600	-0.614// -0.611// -0.600	-0.598// -0.600// -0.600	-0.598// -0.604// -0.600	-0.615// -0.615// -0.600
F_2	-0.629// -0.609// -0.605	-0.617// -0.621// -0.605	-0.622// -0.611// -0.605	-0.615// -0.606// -0.605	-0.656// -0.651// -0.605	-0.608// -0.607// -0.605	-0.608// -0.610// -0.605	-0.612// -0.612// -0.605
F_3	-0.641// -0.613// -0.607	-0.608// -0.623// -0.607	-0.608// -0.608// -0.607	-0.615// -0.607// -0.607	-0.613// -0.601// -0.607	-0.598// -0.617// -0.607	-0.598// -0.581// -0.607	-0.610// -0.610// -0.607
C_2	+0.015// +0.010// -0.031	-0.034// -0.034// -0.031	-0.062// -0.033// -0.031	-0.087// -0.099// -0.031	-0.025// -0.031// -0.031	-0.052// -0.067// -0.031	-0.052// -0.009// -0.031	-0.003// -0.003// -0.031
H_1	+0.150// +0.159// +0.118	+0.130// +0.151// +0.118	+0.133// +0.122// +0.118	+0.131// +0.138// +0.118	+0.146// +0.158// +0.118	+0.118// +0.118// +0.118	+0.118// +0.146// +0.118	+0.091// +0.091// +0.118
H_2	+0.075/ +0.083// +0.129	+0.126// +0.117// +0.129	+0.123// +0.128// +0.129	+0.139// +0.144// +0.129	+0.137// +0.132// +0.129	+0.123// +0.124// +0.129	+0.123// +0.077// +0.129	+0.136// +0.136// +0.129
C_3	+1.016// +0.988// +1.025	+1.049// +1.003// +1.025	+1.015// +1.049// +1.025	+1.037// +1.021// +1.025	+1.000// +1.008// +1.025	+1.000// +0.996// +1.025	+1.000// +1.012// +1.025	+1.013// +1.013// +1.025
F_5	-0.608// -0.618// -0.606	-0.632// -0.613// -0.606	-0.624// -0.618// -0.606	-0.624// -0.615// -0.606	-0.616// -0.619// -0.606	-0.621// -0.623// -0.606	-0.621// -0.618// -0.606	-0.614// -0.614// -0.606
F_6	-0.610// -0.627// -0.620	-0.622// -0.630// -0.620	-0.625// -0.630// -0.620	-0.640// -0.628// -0.620	-0.624// -0.623// -0.620	-0.624// -0.627// -0.620	-0.624// -0.620// -0.620	-0.624// -0.624// -0.620
H_3	+0.139// +0.148// +0.135	+0.143// +0.163// +0.135	+0.174// +0.112// +0.135	+0.147// +0.141// +0.135	+0.115// +0.108// +0.135	+0.208// +0.222// +0.135	+0.208// +0.175// +0.135	+0.136// +0.136// +0.135

Table S2. The dipole moments of HFO-1234ze(E) and HFC-245fa molecules calculated using the Bader analysis algorithm (values in parentheses corresponds to the molecule number presented in Figures 8 and 9, respectively) and the distances between the corresponded molecules and the nearest guests.

System	HFO-1234ze(E)	HFO-1234ze(E) + CH_4
Guest	HFO-1234ze(E) Dipole [D] (mono:1.264D); $d_{HFO\text{-}1234ze(E)\text{-}HFO\text{-}1234ze(E)}$: d_{FF}; d_{HF}; d_{HH} [nm]; $d_{HFO\text{-}1234ze(E)\text{-}CH4}$: d_{FH}; d_{HH} [nm]	
1	1.157; 0.374(1-8); 0.325(1-8); 0.464(1-8)	1.277; 0.375(1-8); 0.325(1-8); 0.466(1-8); 0.449(1-18); 0.415(1-21)
2	1.598; 0.480(2-5); 0.446(2-1); 0.540(2-5)	1.164; 0.483(2-5); 0.446(2-1); 0.541(2-5) 0.375(2-21);0.430(2-9)
3	1.188; 0.280(3-5); 0.443(3-5); 0.485(3-1)	1.341; 0.281(3-5); 0.443(3-5); 0.486(3-1); 0.339(3-10); 0.476(3-22)
4	1.837; 0.280(4-8); 0.305(4-7); 0.482(4-7)	1.665; 0.280(4-8); 0.307(4-7); 0.484(4-7); 0.372(4-22); 0.468(4-10)
5	1.635; 0.280(5-3); 0.443(5-3); 0.540(5-2)	1.560; 0.281(5-3); 0.443(5-3); 0.541(5-2); 0.434(5-24); 0.427(5-20)
6	1.123; 0.375(6-7); 0.341(6-7); 0.494(6-7)	1.181; 0.375(6-7); 0.342(6-7); 0.496(6-7); 0.451(6-16); 0.416(6-23)
7	1.234; 0.375(7-6); 0.305(7-4); 0.482(7-4)	1.550; 0.375(7-6); 0.307(7-4); 0.484(7-4); 0.427(7-21); 0.443(18)
8	1.226; 0.280(8-4); 0.325(8-1); 0.464(8-1)	1.533; 0.280(8-4); 0.325(8-1); 0.466(8-1) 0.388(8-23); 0.440(16)
System	HFC-245fa	HFC-245fa + CH_4
Guest	HFC-245fa Dipole [D] (mono:4.625D);$d_{HFC\text{-}245fa\text{-}HFC\text{-}245fa}$: d_{FF}; d_{HF}; d_{HH} (nm); $d_{HFC\text{-}245fa\text{-}CH4}$: d_{FF}; d_{HF}; d_{HH} (nm)	
1	5.448; 0.292(1-8); 0.345(1-8); 0.483(1-3)	5.486; 0.292(1-8); 0.348(1-8); 0.482(1-3); 0.396(1-16); 0.425(1-21)
2	3.885; 0.391(2-1); 0.494(2-4); 0.493(2-5)	3.907; 0.392(2-1); 0.448(2-1); 0.495(2-5); 0.401(2-23); 0.433(2-9)
3	5.516; 0.282(3-5); 0.411(3-4); 0.483(3-1)	5.337; 0.285(3-5); 0.405(3-4); 0.482(3-1); 0.339(3-10); 0.464(3-22)
4	4.966; 0.288 (4-8); 0.337(4-7); 0.502(4-7)	5.193; 0.289 (4-8); 0.336(4-7); 0.501(4-7); 0.382(3-22); 0.474(4-13)
5	5.204; 0.282(5-3); 0.488(5-8); 0.493(5-2)	5.167; 0.285(5-3); 0.489(5-8); 0.495(5-2);

		0.397(5-24); 0.433(5-20)
6	5.508; 0.382(6-7); 0.345(6-7); 0.495(6-7)	5.630; 0.382(6-7); 0.346(6-7); 0.494(6-7); 0.410(6-13); 0.421(1-23)
7	5.132; 0.382 (7-6); 0.337(7-4); 0.495(7-6)	5.268; 0.382 (7-6); 0.336(7-4); 0.494(7-6); 0.396(7-21); 0.446(7-13)
8	5.580; 0.288(8-4); 0.345(8-1); 0.489 (8-1)	5.680; 0.289(8-4); 0.348(8-1); 0.491(8-1); 0.373(8-23); 0.420(8-16)