Supporting Information

The structure of aqueous solutions of hexafluoro-iso-propanol studied by neutron diffraction with hydrogen/deuterium isotope substitution and empirical potential structure refinement modeling

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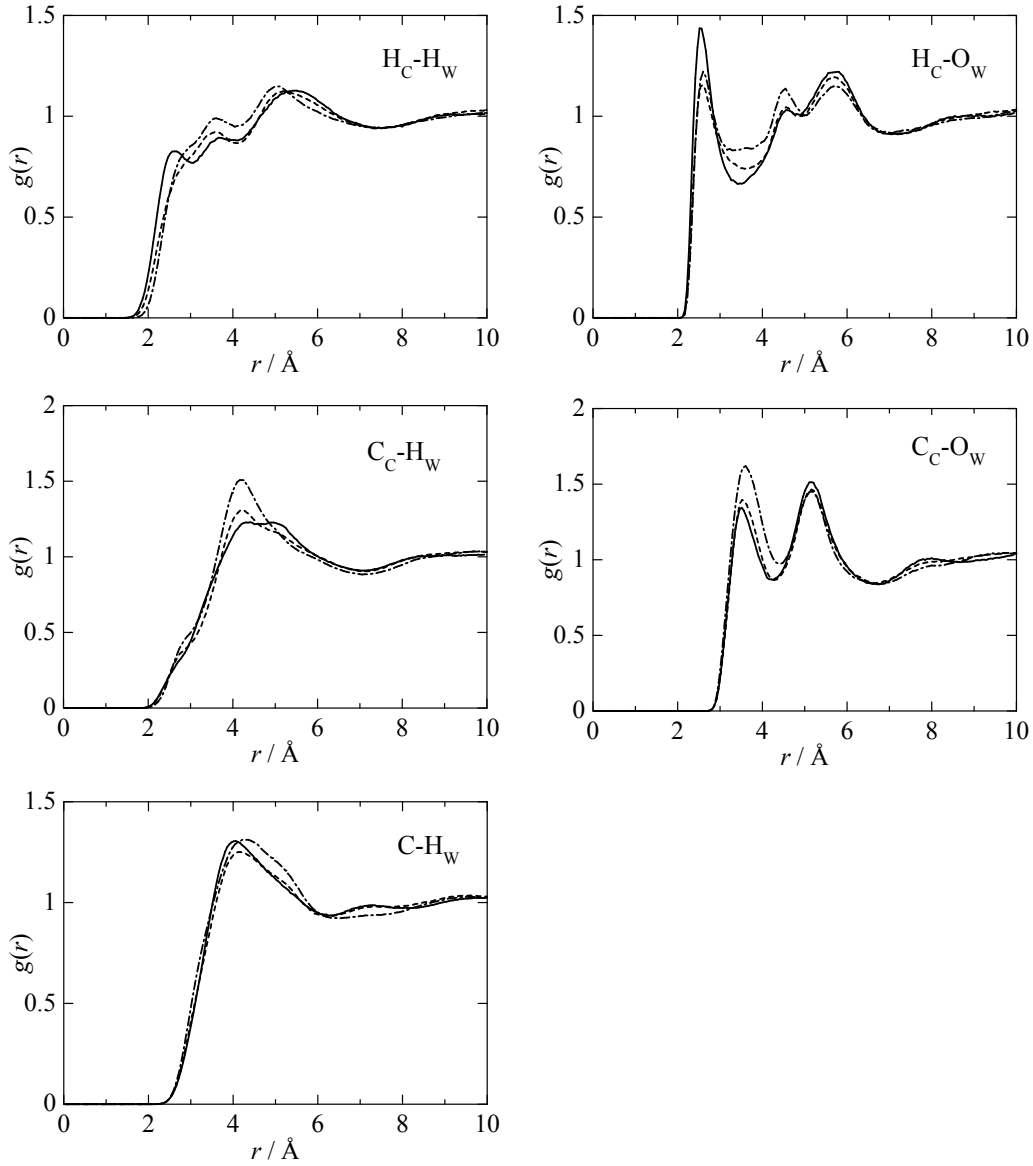

Figure S1. The pair correlation functions of the non-polar interaction between HFIP and water molecules for the HFIP-water mixtures at x_{HFIP}=0.1 (solid lines), 0.2 (dashed lines), and 0.4 (dot and dashed lines).

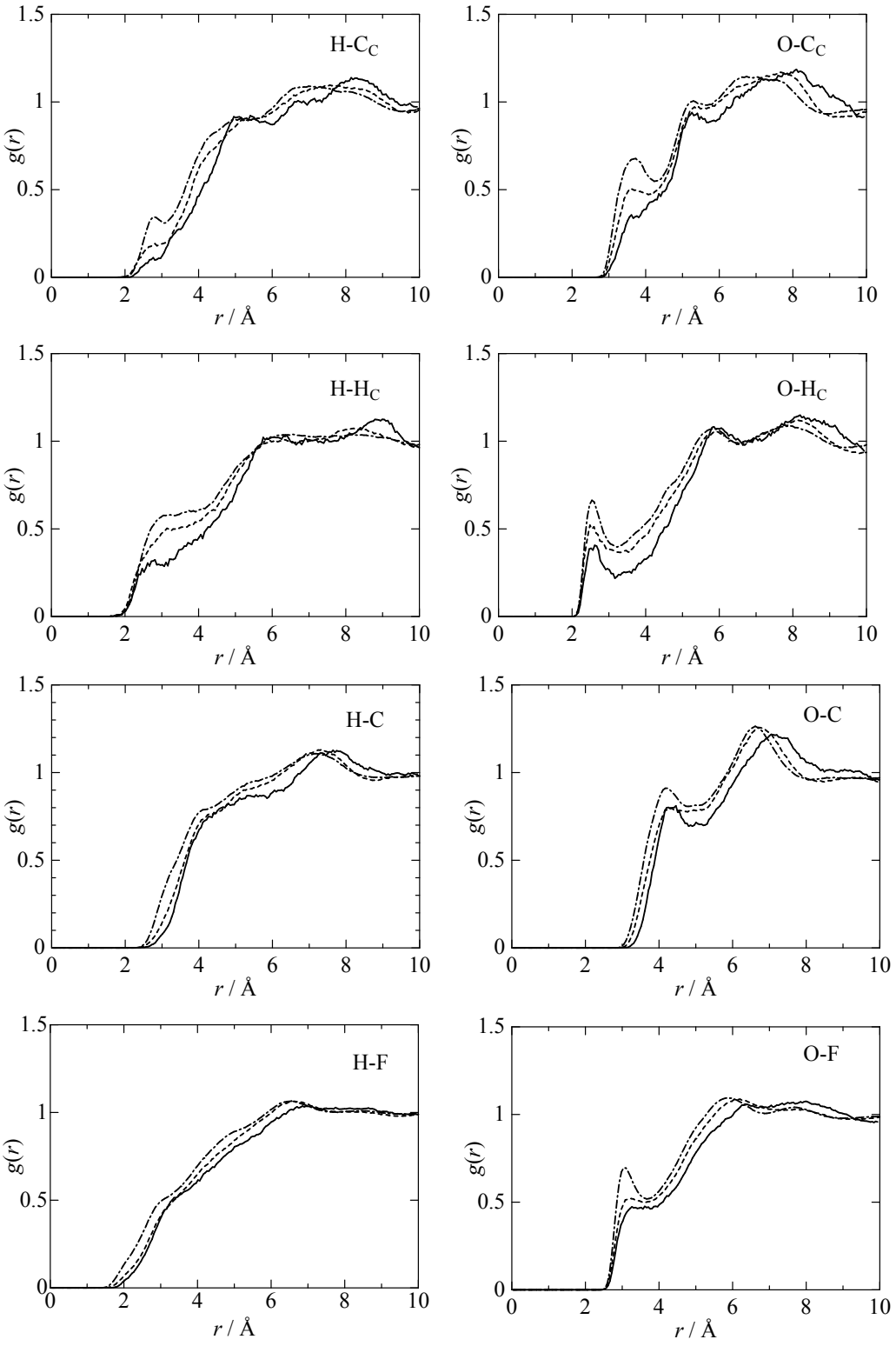

Figure S2. The pair correlation functions of HFIP-HFIP interaction for the HFIP-water mixtures at x_{HFIP}=0.1 (solid lines), 0.2 (dashed lines), and 0.4 (dot and dashed lines).

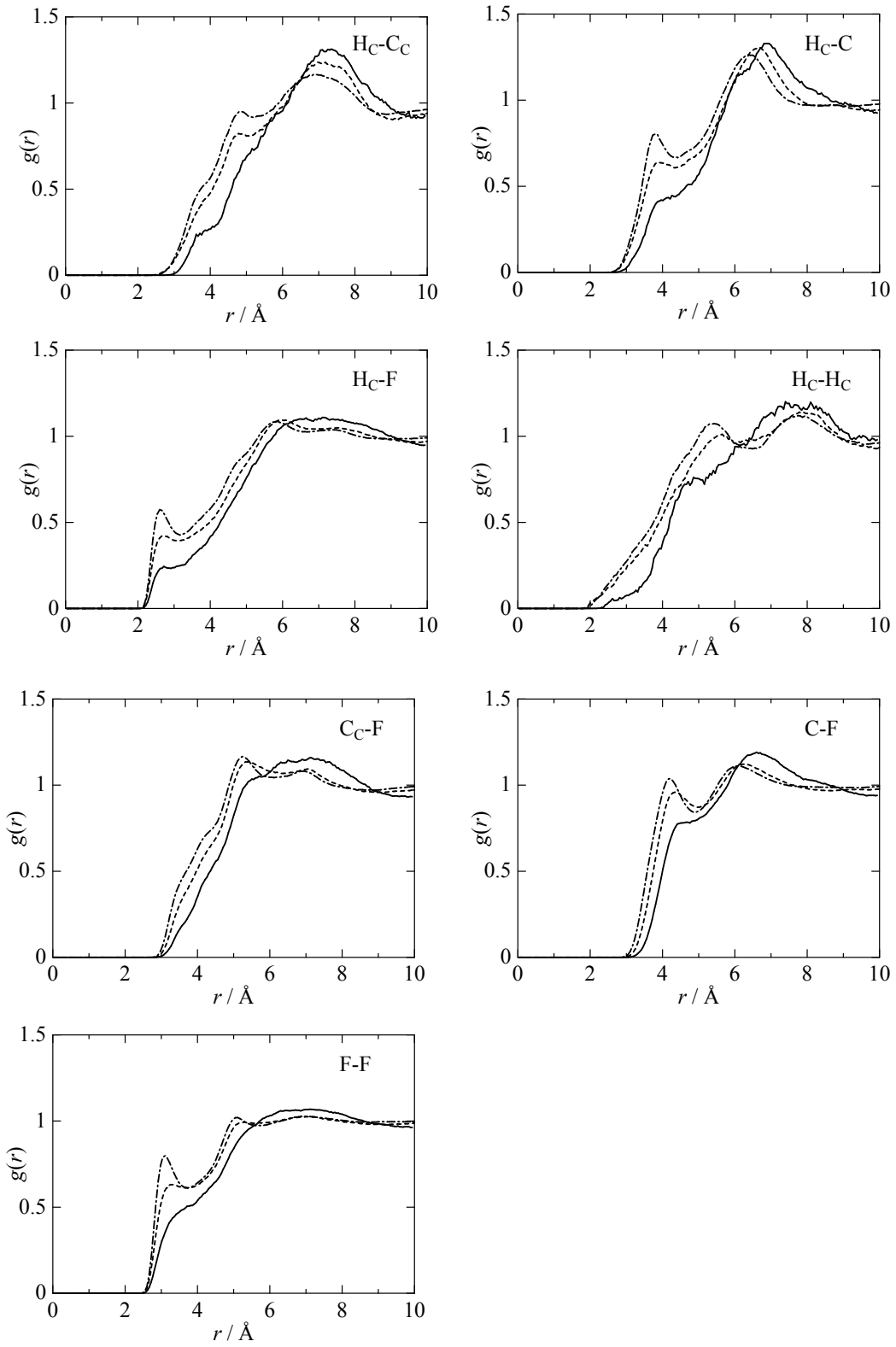

Figure S2. (Continured)

Table S1. The coordination number of the second neighbor coordination shell obtained from integration of pcfs between the lower and upper limits r_{min} and r_{max}, respectively, HFIP-HFIP interactions at x_{HFIP} = 0.1, 0.2, and 0.4.

			x_{HFIP}		
	r_{min}	r_{max}	0.1	0.2	0.4
O_W–O_W	3.3	6.0	15.0 ± 3.2	10.6 ± 3.1	5.4 ± 2.8
O_W–H_W	2.5	4.5	14.5 ± 3.6	11.1 ± 3.6	6.5 ± 3.3
O_W-H	2.5	4.5	0.65 ± 0.75	1.0 ± 0.9	1.6 ± 1.1
O-H_W	2.5	4.0	7.3 ± 2.0	5.5 ± 2.4	3.4 ± 1.9
O-O	3.3	7.0	2.4 ± 1.3	3.6 ± 1.3	5.3 ± 1.5
O-H	2.5	4.0	0.19 ± 0.40	0.34 ± 0.50	0.57 ± 0.70
C-O_W	5.3	7.5	23.5 ± 3.0	15.3 ± 4.0	7.4 ± 2.9
Cc-O_W	4.2	6.0	15.0 ± 2.2	9.8 ± 3.9	4.8 ± 2.5
C_C-H_W	3.3	6.0	35.2 ± 4.4	23.3 ± 7.0	12.3 ± 5.6
C_C-O	4.3	5.0	1.2 ± 0.9	1.8 ± 1.1	2.9 ± 1.5
C_C-H	3.3	6.0	1.2 ± 0.9	1.8 ± 1.1	2.9 ± 1.5
C-C	5.8	8.5	8.6 ± 2.1	12.3 ± 2.5	16.4 ± 2.8
F-C	4.8	8.0	7.7 ± 1.9	11.8 ± 2.5	15.7 ± 2.6
F-F	3.8	5.6	5.2 ± 2.3	9.0 ± 3.1	12.4 ± 3.2