Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary materials for "**Wide-Angle X-ray Diffraction and Molecular Dynamics Study of Medium-range Order in Ambient and Hot Water**" by Huang *et al.*

Table 1S: Tabulated data of S(Q)s shown in Fig.4.

Q(Å^{-1})	7°C	25°C	66°C
0.50	-0.942	-0.939	-0.932
0.60	-0.940	-0.937	-0.929
0.70	-0.935	-0.932	-0.922
0.80	-0.929	-0.927	-0.915
0.90	-0.920	-0.916	-0.904
1.00	-0.906	-0.902	-0.888
1.10	-0.885	-0.882	-0.866
1.20	-0.853	-0.852	-0.836
1.30	-0.806	-0.806	-0.790
1.40	-0.736	-0.740	-0.729
1.50	-0.626	-0.645	-0.641
1.60	-0.481	-0.513	-0.523
1.70	-0.287	-0.339	-0.369
1.80	-0.081	-0.140	-0.192
1.90	0.087	0.040	-0.020
2.00	0.182	0.156	0.122
2.10	0.191	0.188	0.199
2.20	0.160	0.188	0.223
2.30	0.115	0.163	0.226
2.40	0.102	0.141	0.213
2.50	0.103	0.146	0.213
2.60	0.135	0.178	0.223
2.70	0.215	0.225	0.241
2.80	0.303	0.284	0.252
2.90	0.354	0.318	0.248
3.00	0.350	0.296	0.190
3.10	0.270	0.220	0.104
3.20	0.141	0.095	0.007
3.30	-0.005	-0.027	-0.085
3.40	-0.127	-0.124	-0.147
3.50	-0.203	-0.192	-0.193
3.60	-0.236	-0.227	-0.210
3.70	-0.244	-0.225	-0.206
3.80	-0.223	-0.199	-0.183
3.90	-0.191	-0.169	-0.144
4.00	-0.141	-0.123	-0.100
4.10	-0.094	-0.073	-0.043
4.20	-0.039	-0.021	0.008
4.30	0.021	0.041	0.052
4.40	0.067	0.086	0.097
4.50	0.113	0.126	0.130
4.60	0.154	0.159	0.159
4.70	0.168	0.180	0.163
4.80	0.197	0.191	0.176
4.90	0.195	0.193	0.170

5.00	0.178	0.169	0.151
5.10	0.165	0.170	0.127
5.20	0.138	0.137	0.101
5.30	0.097	0.101	0.075
5.40	0.063	0.064	0.041
5.50	0.025	0.024	0.008
5.60	-0.013	-0.009	-0.020
5.70	-0.046	-0.040	-0.047
5.80	-0.072	-0.063	-0.058
5.90	-0.095	-0.076	-0.060
6.00	-0.097	-0.076	-0.065
6.10	-0.087	-0.076	-0.059
6.20	-0.078	-0.061	-0.048
6.30	-0.061	-0.045	-0.028
6.40	-0.032	-0.020	-0.006
6.50	-0.009	0.003	0.015
6.60	0.018	0.034	0.037
6.70	0.041	0.053	0.054
6.80	0.060	0.068	0.072
6.90	0.081	0.074	0.085
7.00	0.088	0.094	0.092
7.10	0.102	0.099	0.082
7.20	0.102	0.097	0.092
7.30	0.097	0.090	0.080
7.40	0.081	0.081	0.066
7.50	0.068	0.068	0.063
7.60	0.056	0.057	0.041
7.70	0.031	0.034	0.033
7.80	0.012	0.008	0.019
7.90	-0.011	-0.007	-0.000
8.00	-0.022	-0.013	-0.010
8.10	-0.035	-0.031	-0.017
8.20	-0.050	-0.035	-0.022
8.30	-0.053	-0.040	-0.031
8.40	-0.052	-0.042	-0.020
8.50	-0.046	-0.048	-0.017
8.60	-0.035	-0.036	-0.011
8.70	-0.030	-0.031	-0.008
8.80	-0.024	-0.019	0.009
8.90	-0.004	0.004	0.007
9.00	0.008	0.006	0.017
9.10	0.016	0.010	0.025
9.20	0.034	0.033	0.028
9.30	0.029	0.037	0.031
9.40	0.040	0.038	0.024
9.50	0.036	0.031	0.025
9.60	0.040	0.033	0.028
9.70	0.033	0.034	0.026
9.80	0.029	0.027	0.014
9.90	0.018	0.015	0.009
10.00	0.014	0.001	0.002
10.10	0.009	0.000	0.002
10.20	-0.004	-0.008	-0.013
10.30	-0.021	-0.012	-0.020

10.40	-0.023	-0.015	-0.022
10.50	-0.024	-0.017	-0.022
10.60	-0.031	-0.010	-0.024
10.70	-0.030	-0.023	-0.022
10.80	-0.027	-0.018	-0.023
10.90	-0.020	-0.018	-0.015
11.00	-0.016	-0.013	-0.012
11.10	-0.017	-0.012	-0.013
11.20	-0.008	0.003	0.003
11.30	0.003	0.010	0.001
11.40	0.006	0.003	0.005
11.50	0.008	0.018	0.013
11.60	0.020	0.016	0.014
11.70	0.020	0.019	0.012
11.80	0.015	0.008	0.019
11.90	0.015	0.021	0.010
12.00	0.011	0.015	0.019
12.10	0.004	0.009	0.012
12.20	0.004	0.008	0.008
12.30	0.004	0.001	0.007
12.40	-0.003	-0.001	0.002
12.50	-0.007	-0.008	-0.003
12.60	-0.010	-0.013	-0.003
12.70	-0.006	-0.010	-0.001
12.80	-0.011	-0.016	-0.004
12.90	-0.017	-0.022	0.001
13.00	-0.015	-0.020	-0.007
13.10	-0.017	-0.014	0.009
13.20	-0.016	-0.009	-0.004
13.30	-0.009	-0.010	-0.001
13.40	-0.009	-0.005	-0.003
13.50	-0.001	-0.004	0.003
13.60	-0.005	-0.001	0.004
13.70	-0.005	0.001	0.000
13.80	0.004	0.001	0.010
13.90	0.008	0.011	0.005
14.00	0.009	0.006	0.002
14.10	0.005	0.010	0.005
14.20	0.014	0.009	0.015
14.30	0.005	0.011	0.013
14.40	0.006	0.007	0.008
14.50	0.012	0.006	0.009
14.60	0.011	0.010	0.017
14.70	0.007	0.010	0.011
14.80	0.011	0.015	0.015
14.90	0.004	-0.001	-0.001
15.00	-0.008	-0.003	-0.002
15.10	-0.009	-0.011	-0.005
15.20	-0.006	-0.008	-0.005
15.30	-0.008	-0.008	-0.010
15.40	-0.005	-0.006	-0.013
15.50	-0.010	-0.016	-0.017
15.60	-0.009	-0.014	-0.018
15.70	-0.016	-0.017	-0.017

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