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Supporting Information

Hydrothermal properties of the COS/D2 water model: A polarizable charge-on-spring water model, at elevated temperatures and pressures

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Table 1. *pVT* and dielectric properties of COS/D2 H_2O, and comparison with SPC/E H_2O and experimental values.*

	COS/D2				SPC/E				Exp.†			
ρ / g/cm^3	P / MPa	κ_T / MPa^{-1}	α_P / °C^{-1}	$\epsilon(0)$	P / MPa	κ_T / MPa^{-1}	α_P / °C^{-1}	$\epsilon(0)$	P / MPa	κ_T / MPa^{-1}	α_P / °C^{-1}	$\epsilon(0)$
						300 °C						
0.001	0.3	3.6	7.2e-4	1	0.3	5.2	2.3e-3	1	0.2	6.0	1.8e-3	1
0.05	9.6	1.6e-1	5.3e-3	1.3	6.8	2.9e-1	1.1e-2	1.6	8.6	–	–	–
0.1	13.7	–	–	1.9	8.0	–	–	2.3	8.6	–	–	–
0.2	13.9	–	–	3.1	6.3	–	–	3.9	8.6	–	–	–
0.3	12.2	–	–	4.7	4.3	–	–	5.7	8.6	–	–	–
0.4	10.7	–	–		2.2	–	–	8.4	8.6	–	–	–
0.5	7.4	–	–	9.4	-1.1	–	–	12.3	8.6	–	–	–
0.6	10.2	–	–	13.3	2.9	–	–	14.9	8.6	–	–	–
0.7	35.0	3.3e-3	3.6e-3	16.9	32.1	2.9e-3	3.0e-3	18.4	8.6	–	–	–
0.8	109	1.1e-3	1.7e-3	20.6	112	1.1e-3	1.5e-3	23.0	73.0	1.2e-3	1.6e-3	24.0
0.9	269	5.1e-4	9.9e-4	24.5	268	5.3e-4	9.2e-4	26.4	231	5.2e-4	9.2e-4	28.7
1.0	560	2.7e-4	6.6e-4	31.0	539	3.0e-4	6.6e-4	31.5	518	2.7e-4	6.1e-4	33.8
						325 °C						
0.001	0.3	3.5	7.0e-4	1	0.3	4.7	2.1e-3	1	0.2	6.0	1.7e-3	1
0.05	10.5	1.3e-1	4.3e-3	1.3	7.9	2.1e-1	8.0e-3	1.6	10.1	1.6e-1	6.0e-3	1.4
0.1	16.0	1.4e-1	1.1e-2	1.8	10.3	–	–	2.2	12.0	–	–	–
0.2	19.2	–	–	3.1	10.5	–	–	3.9	12.0	–	–	–
0.3	18.8	–	–	4.7	9.3	–	–	6.0	12.0	–	–	–
0.4	18.1	–	–	6.7	7.9	–	–	8.5	12.0	–	–	–
0.5	18.6	–	–	9.0	8.8	–	–	11.5	12.0	–	–	–
0.6	27.2	9.5e-3	7.5e-3	11.6	19.3	8.1e-3	5.9e-3	14.1	12.0	–	–	–
0.7	59.6	2.7e-3	2.9e-3	13.9	56.3	2.5e-3	2.6e-3	17.4	28.6	3.0e-3	3.0e-3	18.6
0.8	146	1.0e-3	1.5e-3	19.5	145	1.0e-3	1.4e-3	21.4	107	1.1e-3	1.5e-3	22.7
0.9	317	4.8e-4	9.4e-4	20.8	312	5.1e-4	8.8e-4	25.1	275	4.9e-4	8.8e-4	27.3
1.0	622	2.6e-4	6.4e-4	26.7	594	2.9e-4	6.3e-4	28.1	573	2.7e-4	5.9e-4	32.1
						350 °C (≈ T_c SPC/E)						
0.001	0.3	3.4	6.9e-4	1	0.3	4.3	1.9e-3	1	0.2	6.0	1.6e-3	1
0.05	11.3	1.2e-1	3.8e-3	1.3	8.9	1.7e-1	6.5e-3	1.5	11.1	1.3e-1	4.7e-3	1.3

0.1	18.1	1.0e-1	8.1e-3	1.8	12.5	2.0e-1	1.6e-2	2.2	16.1	1.8e-1	1.6e-2	1.8
0.2	23.8	1.6e-1	2.8e-2	2.9	14.4	1.4	2.2e-1	3.8	16.7	–	–	–
0.3	25.6	2.3e-1	6.3e-2	4.3	14.5	–	–	5.8	16.7	–	–	–
0.4	27.6	1.2e-1	4.7e-2	6.2	15.1	1.8e-1	6.3e-2	8.0	16.7	–	–	–
0.5	31.9	2.6e-2	1.4e-2	8.5	19.2	2.0e-2	1.2e-2	11.2	16.7	–	–	–
0.6	46.7	6.7e-3	5.3e-3	10.9	35.5	6.1e-3	4.5e-3	13.8	20.6	9.9e-3	6.9e-3	13.9
0.7	87.4	2.3e-3	2.5e-3	13.3	79.0	2.2e-3	2.2e-3	17.3	54.6	2.6e-3	2.6e-3	17.6
0.8	183	9.5e-4	1.4e-3	18.0	179	9.4e-4	1.3e-3	19.8	142	9.9e-4	1.3e-3	21.7
0.9	365	4.6e-4	8.9e-4	19.8	355	4.8e-4	8.4e-4	22.9	320	4.7e-4	8.4e-4	25.9
1.0	683	2.5e-4	6.1e-4	25.2	649	2.8e-4	6.1e-4	26.3	628	2.6e-4	5.7e-4	30.6
						375 °C (≈ T_c real + 0.9 °C)						
0.001	0.3	3.3	6.7e-4	1	0.3	4.1	1.8e-3	1	0.2	6.0	1.6e-3	1
0.05	12.2	1.0e-1	3.3e-3	1.3	9.8	1.4e-1	5.4e-3	1.5	11.8	1.1e-1	3.8e-3	1.3
0.1	20.1	8.1e-2	6.4e-3	1.8	14.5	1.3e-1	1.1e-2	2.1	17.9	1.2e-1	9.8e-3	1.8
0.2	28.4	8.7e-2	1.6e-2	2.9	18.5	2.3e-1	3.7e-2	3.7	22.0	4.2e-1	7.8e-2	3.1
0.3	32.7	8.5e-2	2.4e-2	4.4	20.6	1.8e-1	4.2e-2	5.7	22.3	7.0	1.9	4.9
0.4	37.4	4.7e-2	1.8e-2	6.5	24.1	5.1e-2	1.7e-2	7.9	22.5	5.6e-1	1.8e-1	7.2
0.5	45.7	1.6e-2	8.7e-3	8.6	32.5	1.5e-2	7.2e-3	10.3	24.7	3.7e-2	1.7e-2	10.1
0.6	66.3	5.2e-3	4.1e-3	11.2	54.6	4.9e-3	3.5e-3	13.2	37.7	7.0e-3	5.0e-3	13.3
0.7	116	2.0e-3	2.2e-3	14.0	108	1.9e-3	2.0e-3	17.2	79.2	2.2e-3	2.3e-3	16.9
0.8	221	8.8e-4	1.3e-3	16.8	212	8.9e-4	1.2e-3	19.2	177	9.2e-4	1.3e-3	20.7
0.9	414	4.3e-4	8.5e-4	20.4	398	4.6e-4	8.1e-4	22.3	364	4.5e-4	8.0e-4	24.7
1.0	744	2.4e-4	5.9e-4	23.1	705	2.6e-4	5.8e-4	24.5	684	2.5e-4	5.5e-4	29.2
						400 °C						
0.001	0.3	3.1	6.3e-4	1	0.3	3.7	1.6e-3	1	0.2	6.0	1.5e-3	1
0.05	13.0	9.4e-2	3.0e-3	1.3	10.8	1.3e-1	4.8e-3	1.5	12.6	1.0e-1	3.3e-3	1.3
0.1	22.0	6.9e-2	5.4e-3	1.7	16.6	1.1e-1	8.9e-3	2.1	20.0	9.0e-2	7.0e-3	1.8
0.2	32.8	6.1e-2	1.1e-2	2.7	22.6	1.2e-1	1.9e-2	3.5	26.5	1.4e-1	2.4e-2	3.0
0.3	39.8	4.8e-2	1.3e-2	4.1	37.0	7.1e-2	1.7e-2	5.4	29.0	1.6e-1	4.3e-2	4.7
0.4	47.5	2.7e-2	1.0e-2	5.9	33.3	2.9e-2	9.8e-3	7.6	31.5	7.2e-2	2.6e-2	7.0
0.5	60.7	1.1e-2	6.1e-3	7.9	46.0	1.1e-2	5.3e-3	10.1	37.9	1.8e-2	9.5e-3	9.7
0.6	87.7	4.3e-3	3.4e-3	10.2	74.4	4.1e-3	3.0e-3	12.6	56.8	5.5e-3	4.1e-3	12.7
0.7	145	1.7e-3	2.0e-3	12.7	134	1.8e-3	1.8e-3	15.0	106.0	2.0e-3	2.0e-3	16.1
0.8	258	8.2e-4	1.2e-3	15.6	246	8.4e-4	1.1e-3	18.3	211	8.6e-4	1.2e-3	19.8

0.9	463	4.2e-4	8.1e-4	19.1	442	4.4e-4	7.7e-4	21.2	409	4.3e-4	7.6e-4	23.7
1.0	806	2.3e-4	5.7e-4	23.7	760	2.6e-4	5.6e-4	25.5	740	2.4e-4	5.3e-4	28.0
						425 °C						
0.001	0.3	2.8	5.7e-4	1	0.3	3.5	1.6e-3	1	0.3	2.9e0	1.4e-3	1
0.05	13.8	8.8e-2	2.8e-3	1.3	11.7	1.1e-1	4.2e-3	1.5	13.3	9.4e-2	2.9e-3	1.3
0.1	23.8	6.3e-2	4.9e-3	1.6	18.5	8.8e-2	7.3e-3	2.1	21.9	7.5e-2	5.6e-3	1.7
0.2	37.1	4.6e-2	8.3e-3	2.6	26.6	7.9e-2	1.3e-2	3.5	30.7	8.6e-2	1.5e-2	2.9
0.3	46.4	3.3e-2	9.1e-3	4.0	33.2	4.7e-2	1.1e-2	5.2	35.4	7.8e-2	2.0e-2	4.6
0.4	56.9	2.1e-2	8.0e-3	5.6	42.3	2.1e-2	7.1e-3	7.1	40.4	3.9e-2	1.5e-2	6.7
0.5	73.3	9.6e-3	5.2e-3	7.5	59.1	8.6e-3	4.3e-3	9.4	50.2	1.3e-2	7.1e-3	9.2
0.6	105	3.8e-3	3.0e-3	9.6	92.9	3.6e-3	2.6e-3	12.2	75.0	4.5e-3	3.4e-3	12.2
0.7	168	1.6e-3	1.7e-3	12.0	159	1.6e-3	1.6e-3	14.2	131	1.8e-3	1.8e-3	15.4
0.8	295	7.5e-4	1.1e-3	14.9	280	7.9e-4	1.1e-3	16.6	245	8.1e-4	1.1e-3	18.9
0.9	511	4.1e-4	7.9e-4	18.1	486	4.3e-4	7.4e-4	19.5	452	4.1e-4	7.3e-4	22.7
1.0	870	2.5e-4	6.1e-4	21.3	815	2.5e-5	5.5e-4	22.6	794	2.4e-4	5.1e-4	26.8
						450 °C						
0.001	0.3	3.1	6.2e-4	1	0.3	3.3	1.5e-3	1	0.3	3.0e0	1.4e-3	1
0.05	14.5	7.9e-2	2.6e-3	1.3	12.6	1.0e-1	3.8e-3	1.4	14.1	8.6e-2	2.6e-3	1.3
0.1	25.5	5.1e-2	4.0e-3	1.6	20.4	7.4e-2	6.1e-3	2.0	23.7	6.4e-2	4.6e-3	1.7
0.2	41.2	3.8e-2	6.9e-3	2.5	30.7	5.8e-2	9.5e-3	3.3	34.9	6.1e-2	1.0e-2	2.8
0.3	53.6	2.8e-2	7.8e-3	3.5	39.7	3.5e-2	8.3e-3	4.9	41.9	4.9e-2	1.3e-2	4.4
0.4	67.2	1.5e-2	5.9e-3	4.8	51.7	1.6e-2	5.5e-3	6.8	49.8	2.6e-2	9.8e-3	6.4
0.5	88.1	7.0e-3	3.8e-3	5.8	72.4	7.1e-3	3.5e-3	9.0	63.6	1.0e-2	5.5e-3	8.9
0.6	129	3.1e-3	2.5e-3	9.2	112	3.2e-3	2.3e-3	11.3	93.5	3.9e-3	2.9e-3	11.7
0.7	201	1.5e-3	1.6e-3	11.5	185	1.5e-3	1.5e-3	13.7	157	1.6e-3	1.7e-3	14.8
0.8	332	7.3e-4	1.1e-3	12.9	314	7.5e-4	1.0e-3	15.7	279	7.7e-4	1.0e-2	18.2
0.9	559	3.8e-4	7.4e-4	17.2	529	4.1e-4	7.1e-4	18.4	498	4.0e-4	7.0e-4	21.8
1.0	927	2.1e-4	5.2e-4	19.3	869	2.4e-4	5.3e-4	21.5	855	2.3e-4	4.9e-4	25.9

* Entries marked by a dash (–) correspond to *pVT* points characterized by two-phase (liquid+vapor) coexistence.

† Calculated according to the IAPWS equations[1,2]

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