Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Self-assembling, Reactivity and Molecular Dynamics of Fullerenol Nanoparticles

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Table 1. Density (d), apparent molar volume (V_ϕ), and partial molar volume (V_i) at different temperatures and molality of fullerenol (m) compositions of the {fullerenol (2) + H_2O (1)} mixtures at p = 0.1 MPa.

m [mol·kg^{-1}]	d [g·cm^{-3}]	V_1 [cm^3·mol^{-1}]	V_2 [cm^3·mol^{-1}]	V_ϕ [cm^3·mol^{-1}]
		T = 293.15 K		
0.00000[a]	0.99821			
0.00088	0.99868	18.032	592.36	596.35
0.00283	0.99974	18.033	578.25	585.73
0.00363	1.00018	18.033	574.64	583.11
0.00447	1.00065	18.033	569.85	579.21
0.00692	1.00201	18.034	562.71	574.21
0.00897	1.00317	18.035	556.13	568.94
0.01065	1.00411	18.036	553.24	566.88
0.01311	1.00552	18.037	546.89	561.91
		T = 295.15 K		
0.00000[a]	0.99777			
0.00088	0.99823	18.040	597.38	601.83
0.00283	0.99929	18.041	580.60	589.08
0.00363	0.99973	18.041	576.05	585.65
0.00447	1.00019	18.041	572.82	583.49
0.00692	1.00155	18.042	563.72	576.89
0.00897	1.00270	18.043	557.32	572.09
0.01065	1.00365	18.044	552.76	568.66
0.01311	1.00507	18.046	545.03	562.45
		T = 298.15 K		
0.00000[a]	0.99705			
0.00088	0.99751	18.053	602.36	607.20
0.00283	0.99856	18.054	582.84	592.28
0.00363	0.99899	18.054	580.09	590.85
0.00447	0.99946	18.054	573.41	585.39
0.00692	1.00082	18.056	563.09	577.94
0.00897	1.00196	18.057	557.18	573.95
0.01065	1.00291	18.058	552.05	569.89
0.01311	1.00433	18.059	543.67	563.60
		T = 303.15 K		
0.00000[a]	0.99565			
0.00088	0.99609	18.079	622.38	629.45
0.00283	0.99711	18.080	595.55	609.50
0.00363	0.99754	18.080	588.19	604.11
0.00447	0.99799	18.080	582.76	600.56
0.00692	0.99933	18.082	568.16	590.39
0.00897	1.00048	18.084	557.00	582.26

0.01065	1.00143	18.085	549.61	577.02
0.01311	1.00285	18.087	538.69	569.00
		T = 309.15 K		
0.00000[a]	0.99369			
0.00088	0.99409	18.115	661.17	674.91
0.00283	0.99504	18.116	622.13	648.24
0.00363	0.99545	18.117	609.94	639.73
0.00447	0.99590	18.117	596.08	629.30
0.00692	0.99723	18.120	568.51	610.05
0.00897	0.99838	18.123	549.84	597.17
0.01065	0.99933	18.125	537.85	589.36
0.01311	1.00080	18.130	517.79	574.86
		T = 310.15 K		
0.00000[a]	0.99333			
0.00088	0.99372	18.121	670.79	686.16
0.00283	0.99464	18.123	633.09	662.55
0.00363	0.99504	18.123	620.08	653.68
0.00447	0.99550	18.124	600.90	638.31
0.00692	0.99682	18.127	570.52	617.27
0.00897	0.99795	18.130	551.68	604.99
0.01065	0.99892	18.133	535.99	593.98
0.01311	1.00041	18.138	512.74	577.01
		T = 313.15 K		
0.00000[a]	0.99222			
0.00088	0.99254	18.142	739.42	766.94
0.00283	0.99338	18.144	665.69	716.55
0.00363	0.99378	18.145	637.95	695.70
0.00447	0.99419	18.147	619.57	683.83
0.00692	0.99548	18.152	570.89	650.72
0.00897	0.99665	18.157	535.12	626.23
0.01065	0.99765	18.162	509.70	608.85
0.01311	0.99918	18.169	475.89	585.80

[a]reference[32])

Table 2. Viscosity (η) of {fullerenol+ H_2O} binary mixture as a function of fullerenol molality (m) in the temperature range from (293.15 to 313.15) K at p = 0.1 MPa.

m [mol·kg^{-1}]	*T* [K]					
	293.15	298.15	303.15	309.15	310.15	313.15
	η [mPa·s]					
0.00000[a]	1.003	0.890	0.797	0.719	0.691	0.653
0.00450	1.236	1.112	1.057	0.974	0.970	0.960
0.00523	1.248	1.124	1.071	0.989	0.986	0.972
0.00680	1.269	1.144	1.090	1.010	1.006	0.990
0.01150	1.315	1.192	1.137	1.050	1.043	1.020
0.01450	1.332	1.205	1.165	1.073	1.066	1.033
0.01724	1.347	1.222	1.180	1.091	1.081	1.044
0.02500	1.373	1.256	1.214	1.130	1.113	1.056
0.03724	1.404	1.301	1.269	1.159	1.140	1.074

[a]reference[32])

Table 3. Masson's equation fitting parameters for the {fullerenol + H_2O} solutions in the temperature range from (293.15 to 313.15) K with the deviations of their fit (σ) and regression coefficient (R^2).

T [K]	V_ϕ^o [cm^3·mol^{-1}]	S_v [cm$^{9/2}$·mol$^{-3/2}$]	R^2
293.15	607.31	-401.07	0.9993
295.15	613.73	-446.79	0.9991
298.15	620.33	-499.82	0.9992
303.15	647.76	-696.28	0.9994
309.15	710.38	-1104.42	0.9991
310.15	728.92	-1324.20	0.9992
313.15	828.41	-2148.10	0.9989

Table 4. Electrical conductivity of {fullerenol + H_2O} binary mixtures as a function of fullerenol molality in the temperature range from (293.15 to 313.15) K and at p = 0.1 MPa.

m [mol·kg^{-1}]	T [K]					
	293.15	298.15	303.15	309.15	310.15	313.15
	κ [mS·cm^{-1}]					
0.00098	0.046	0.054	0.060	0.070	0.077	0.082
0.00150	0.068	0.079	0.089	0.104	0.113	0.121
0.00295	0.127	0.148	0.167	0.193	0.206	0.218
0.00537	0.215	0.252	0.284	0.328	0.345	0.357
0.01046	0.391	0.457	0.521	0.595	0.623	0.649
0.01927	0.682	0.784	0.890	1.021	1.060	1.117
0.02645	0.896	1.030	1.162	1.326	1.382	1.453
0.03431	1.107	1.268	1.434	1.609	1.684	1.805
0.04122	1.291	1.469	1.660	1.855	1.950	2.103
0.04894	1.507	1.698	1.918	2.131	2.223	2.423

Table 5. Jones–Dole's equation fitting parameters for the viscosity of {fullerenol+ H_2O} solutions in the temperature range from (293.15 to 313.15) K with the deviations of their fit (σ) and regression coefficient (R^2).

T [K]	A [dm$^{3/2}$·mol$^{-1/2}$]	B [dm^3·mol^{-1}]	R^2
293.15	4.166	-11.36	0.9991
298.15	4.414	-11.60	0.9993
303.15	6.085	-19.05	0.9989
309.15	7.240	-23.51	0.9986
310.15	7.655	-24.90	0.9984
313.15	8.797	-29.80	0.9977

Table 6. Molar conductivity of {fullerenol + H_2O} binary mixtures as a function of fullerenol molality in the temperature range from (293.15 to 313.15) K and at p = 0.1 MPa.

m [mol·kg^{-1}]	T [K]					
	293.15	298.15	303.15	309.15	310.15	313.15
	Λ [S·cm^2·mol^{-1}]					
0.00000	54.08	62.82	70.62	82.27	92.36	101.41
0.00098	48.87	57.19	64.34	74.70	81.88	88.10
0.00150	47.30	54.98	62.02	72.06	78.62	84.09
0.00295	44.83	52.12	58.96	68.14	72.80	77.15
0.00537	41.60	48.89	55.21	63.83	67.15	69.51
0.01046	38.95	45.62	52.12	59.61	62.43	65.10
0.01927	37.12	42.71	48.57	55.83	57.95	61.20
0.02645	35.64	41.02	46.37	53.02	55.27	58.21
0.03431	34.10	39.12	44.29	49.80	52.15	55.98
0.04122	33.24	37.86	42.84	47.97	50.45	54.48
0.04894	32.80	37.00	41.88	46.62	48.64	53.09

[a] values obtained using equation $\Lambda = \kappa/c$)

Table 7. Values of the limiting apparent molar expansibilities at different temperatures

T [K]	293.15	295.15	298.15	303.15	309.15	310.15	313.15
E_Φ^o [cm^3·mol^{-1}·K^{-1}]	-5.15	-2.18	2.27	9.68	18.58	20.06	24.51

Table 8. Bond lengths [Å] comparison for C_{60} as obtained by DFT and OPLS_2005

		DFT	OPLS_2005			DFT	OPLS_2005
C1	C2	1.4531	1.4106	C1	C6	1.3924	1.4186
C1	C7	1.4508	1.4102	C2	C3	1.3928	1.4177
C2	C9	1.4500	1.4099	C3	C4	1.4513	1.4103
C3	C11	1.4532	1.4082	C4	C5	1.3941	1.4190
C4	C12	1.4513	1.4110	C5	C6	1.4528	1.4103
C5	C15	1.4509	1.4113	C6	C17	1.4524	1.4087
C7	C8	1.4525	1.4080	C7	C19	1.3959	1.4179
C8	C9	1.4525	1.4069	C8	C20	1.3915	1.4174
C9	C10	1.3949	1.4166	C10	C57	1.4515	1.4072
C10	C59	1.4535	1.4087	C11	C29	1.4512	1.4060
C11	C59	1.3946	1.4164	C12	C13	1.3926	1.4169
C12	C29	1.4531	1.4081	C13	C14	1.4514	1.4075
C13	C39	1.4506	1.4085	C14	C15	1.3935	1.4174
C14	C28	1.4511	1.4095	C15	C16	1.4525	1.4093
C16	C17	1.4511	1.4075	C16	C26	1.3923	1.4172
C17	C18	1.3955	1.4177	C18	C19	1.4542	1.4089
C18	C24	1.4545	1.4087	C19	C22	1.4543	1.4109
C20	C21	1.4508	1.4077	C20	C56	1.4518	1.4087
C21	C22	1.3953	1.4167	C21	C54	1.4512	1.4095
C22	C23	1.4543	1.4087	C23	C24	1.4541	1.4064
C23	C52	1.3959	1.4168	C24	C25	1.3954	1.4170

C25	C26	1.4510	1.4077	C25	C50	1.4521	1.4085
C26	C27	1.4529	1.4093	C27	C28	1.3939	1.4169
C27	C49	1.4511	1.4096	C28	C38	1.4534	1.4096
C29	C58	1.3945	1.4162	C30	C31	1.3953	1.4170
C30	C37	1.4537	1.4077	C30	C60	1.4525	1.4115
C31	C32	1.4549	1.4079	C31	C40	1.4519	1.4083
C32	C33	1.3953	1.4179	C32	C41	1.4553	1.4097
C33	C34	1.4539	1.4091	C33	C44	1.4535	1.4113
C34	C46	1.4523	1.4072	C34	C60	1.3946	1.4192
C35	C36	1.4506	1.4078	C35	C48	1.3934	1.4167
C35	C60	1.4530	1.4120	C36	C37	1.4524	1.4060
C36	C49	1.3936	1.4173	C37	C38	1.3938	1.4175
C38	C39	1.4520	1.4087	C39	C40	1.3939	1.4177
C40	C58	1.4529	1.4083	C41	C42	1.3970	1.4174
C41	C58	1.4546	1.4094	C42	C43	1.4551	1.4077
C42	C59	1.4555	1.4105	C43	C44	1.3960	1.4164
C43	C57	1.4532	1.4077	C44	C45	1.4551	1.4095
C45	C46	1.4522	1.4067	C45	C55	1.3946	1.4165
C46	C47	1.3943	1.4164	C47	C48	1.4507	1.4076
C47	C53	1.4525	1.4087	C48	C51	1.4534	1.4095
C49	C50	1.4529	1.4086	C50	C51	1.3930	1.4179
C51	C52	1.4514	1.4088	C52	C53	1.4531	1.4079
C53	C54	1.3920	1.4174	C54	C55	1.4536	1.4090
C55	C56	1.4507	1.4080	C56	C57	1.3933	1.4176
RMSE = 0.0382 Å							

Table 9. Bond lengths [Å] comparison for $C_{60}(OH)_{24}$ as obtained by DFT and OPLS_2005

		DFT	OPLS_2005			DFT	OPLS_2005
C1	C2	1.5348	1.5287	C1	C5	1.5202	1.5148
C1	C9	1.5060	1.5209	C1	O61	1.4385	1.4109
C2	C3	1.5375	1.5298	C2	C12	1.3374	1.3537
C3	C4	1.5266	1.5130	C3	C15	1.5032	1.5225
C3	O62	1.4313	1.4110	C4	C5	1.3365	1.3371
C4	C18	1.5072	1.5221	C5	C6	1.5103	1.5239
C6	C7	1.5267	1.5129	C6	C20	1.5316	1.5283
C6	O63	1.4320	1.4106	C7	C8	1.5058	1.5224
C7	C22	1.3357	1.3373	C8	C9	1.5278	1.5121
C8	C25	1.5374	1.5289	C8	O64	1.4308	1.4110
C9	C10	1.3352	1.3359	C10	C11	1.5049	1.5206
C10	C26	1.5254	1.5137	C11	C12	1.5389	1.5288
C11	C29	1.5234	1.5147	C11	O65	1.4321	1.4101
C12	C13	1.5322	1.5289	C13	C14	1.5094	1.5230
C13	C30	1.5249	1.5139	C13	O66	1.4299	1.4097
C14	C15	1.3349	1.3372	C14	C33	1.5253	1.5138
C15	C16	1.5261	1.5139	C16	C17	1.5110	1.5241
C16	C34	1.5321	1.5279	C16	O67	1.4308	1.4107
C17	C18	1.5219	1.5161	C17	C37	1.3368	1.3381
C18	C19	1.5337	1.5278	C18	O68	1.4373	1.4113
C19	C20	1.3368	1.3530	C19	C38	1.5373	1.5282

C20	C21	1.5376	1.5279	C21	C22	1.5258	1.5161
C21	C40	1.5051	1.5214	C21	O69	1.4296	1.4104
C22	C23	1.5068	1.5241	C23	C24	1.5362	1.5269
C23	C42	1.5250	1.5133	C23	O70	1.4303	1.4101
C24	C25	1.3353	1.3527	C24	C44	1.5320	1.5282
C25	C26	1.5312	1.5286	C26	C27	1.5097	1.5236
C26	O71	1.4321	1.4098	C27	C28	1.5253	1.5143
C27	C45	1.3368	1.3380	C28	C29	1.5052	1.5254
C28	C47	1.5372	1.5280	C28	O72	1.4314	1.4103
C29	C30	1.3350	1.3372	C30	C31	1.5055	1.5213
C31	C32	1.5259	1.5159	C31	C48	1.5375	1.5277
C31	O73	1.4293	1.4104	C32	C33	1.5063	1.5240
C32	C50	1.3357	1.3371	C33	C34	1.5361	1.5271
C33	O74	1.4303	1.4101	C34	C35	1.3359	1.3528
C35	C36	1.5312	1.5286	C35	C51	1.5373	1.5292
C36	C37	1.5100	1.5235	C36	C53	1.5254	1.5132
C36	O75	1.4321	1.4098	C37	C38	1.5251	1.5145
C38	C39	1.5047	1.5255	C38	O76	1.4315	1.4103
C39	C40	1.3348	1.3373	C39	C54	1.5238	1.5151
C40	C41	1.5251	1.5141	C41	C42	1.5093	1.5229
C41	C55	1.5319	1.5284	C41	O77	1.4299	1.4097
C42	C43	1.3350	1.3372	C43	C44	1.5252	1.5139
C43	C60	1.5034	1.5225	C44	C45	1.5115	1.5238
C44	O78	1.4307	1.4107	C45	C46	1.5223	1.5163
C46	C47	1.5334	1.5280	C46	C59	1.5072	1.5220
C46	O79	1.4374	1.4113	C47	C48	1.3366	1.3530
C48	C49	1.5315	1.5285	C49	C50	1.5268	1.5131
C49	C58	1.5111	1.5239	C49	O80	1.4325	1.4106
C50	C51	1.5061	1.5221	C51	C52	1.5270	1.5118
C51	O81	1.4307	1.4110	C52	C53	1.3352	1.3357
C52	C57	1.5063	1.5207	C53	C54	1.5044	1.5204
C54	C55	1.5387	1.5288	C54	O82	1.4322	1.4101
C55	C56	1.3374	1.3537	C56	C57	1.5350	1.5284
C56	C60	1.5377	1.5296	C57	C58	1.5208	1.5150
C57	O83	1.4377	1.4109	C58	C59	1.3368	1.3371
C59	C60	1.5270	1.5132	C60	O84	1.4313	1.4110
O61	H85	0.9688	0.9503	O62	H86	0.9690	0.9510
O63	H87	0.9706	0.9511	O64	H88	0.9694	0.9519
O65	H89	0.9695	0.9506	O66	H90	0.9708	0.9526
O67	H91	0.9702	0.9505	O68	H92	0.9691	0.9504
O69	H93	0.9693	0.9500	O70	H94	0.9698	0.9507
O71	H95	0.9707	0.9522	O72	H96	0.9694	0.9505
O73	H97	0.9693	0.9500	O74	H98	0.9698	0.9507
O75	H99	0.9707	0.9522	O76	H100	0.9695	0.9505
O77	H10	0.9708	0.9526	O78	H102	0.9702	0.9505
O79	H10	0.9691	0.9504	O80	H104	0.9706	0.9511
O81	H10	0.9694	0.9519	O82	H106	0.9695	0.9506
O83	H10	0.9689	0.9503	O84	H108	0.9690	0.9510
RMSE = 0.0152 Å							

Table 10. Bond angles [°] comparison for C_{60} as obtained by DFT and OPLS_2005

			DFT	OPLS_2005				DFT	OPLS_2005
C6	C1	C2	120.17	119.98	C7	C1	C2	108.17	107.83
C7	C1	C6	120.04	120.00	C3	C2	C1	120.23	119.95
C9	C2	C1	108.03	107.83	C9	C2	C3	119.87	119.94
C4	C3	C2	119.63	120.11	C11	C3	C2	119.93	119.86
C11	C3	C4	108.07	107.69	C5	C4	C3	120.17	119.96
C12	C4	C3	107.93	108.26	C12	C4	C5	120.21	119.71
C6	C5	C4	120.19	119.94	C15	C5	C4	120.10	119.78
C15	C5	C6	107.99	108.29	C5	C6	C1	119.61	120.07
C17	C6	C1	119.70	120.02	C17	C6	C5	108.12	107.71
C8	C7	C1	107.71	108.26	C19	C7	C1	120.33	119.96
C19	C7	C8	120.47	120.23	C9	C8	C7	108.26	107.78
C20	C8	C7	119.65	119.93	C20	C8	C9	119.62	120.27
C8	C9	C2	107.83	108.31	C10	C9	C2	120.21	120.29
C10	C9	C8	120.45	119.65	C57	C10	C9	119.68	120.43
C59	C10	C9	120.09	119.56	C59	C10	C57	107.84	107.59
C29	C11	C3	107.96	108.17	C59	C11	C3	120.38	120.02
C59	C11	C29	120.07	120.11	C13	C12	C4	119.63	120.38
C29	C12	C4	108.08	107.62	C29	C12	C13	119.80	119.84
C14	C13	C12	120.21	119.94	C39	C13	C12	120.07	120.02
C39	C13	C14	108.09	107.62	C15	C14	C13	120.15	119.81
C28	C14	C13	107.97	108.17	C28	C14	C15	120.22	119.71
C14	C15	C5	119.70	120.38	C16	C15	C5	107.88	107.64
C16	C15	C14	119.78	119.95	C17	C16	C15	108.23	108.19
C26	C16	C15	120.05	120.44	C26	C16	C17	119.97	119.81
C16	C17	C6	107.78	108.18	C18	C17	C6	120.46	119.94
C18	C17	C16	120.26	120.28	C19	C18	C17	119.72	120.10
C24	C18	C17	119.78	119.82	C24	C18	C19	108.01	107.72
C18	C19	C7	119.74	119.97	C22	C19	C7	119.75	119.58
C22	C19	C18	107.96	108.29	C21	C20	C8	120.09	120.12
C56	C20	C8	120.12	119.80	C56	C20	C21	108.23	107.60
C22	C21	C20	120.38	119.81	C54	C21	C20	107.69	108.15
C54	C21	C22	120.48	119.66	C21	C22	C19	119.66	120.33
C23	C22	C19	108.06	107.63	C23	C22	C21	119.65	119.88
C24	C23	C22	107.95	108.21	C52	C23	C22	119.72	120.40
C52	C23	C24	119.77	119.71	C23	C24	C18	108.02	108.15
C25	C24	C18	119.76	119.94	C25	C24	C23	119.68	120.17
C26	C25	C24	120.32	120.14	C50	C25	C24	120.52	119.86
C50	C25	C26	107.84	107.61	C25	C26	C16	119.90	120.00
C27	C26	C16	120.12	119.50	C27	C26	C25	108.24	108.19
C28	C27	C26	119.85	120.19	C49	C27	C26	107.81	108.10
C49	C27	C28	119.67	119.67	C27	C28	C14	119.97	120.21
C38	C28	C14	108.01	108.13	C38	C28	C27	120.35	119.63
C12	C29	C11	107.96	108.25	C58	C29	C11	120.11	120.16
C58	C29	C12	120.34	119.98	C37	C30	C31	120.34	120.53
C60	C30	C31	120.14	119.45	C60	C30	C37	108.00	107.70
C32	C31	C30	120.11	120.36	C40	C31	C30	119.59	119.20
C40	C31	C32	107.89	108.03	C33	C32	C31	119.65	119.96
C41	C32	C31	108.09	108.01	C41	C32	C33	119.86	119.75

C34	C33	C32	120.22	120.10	C44	C33	C32	120.26	119.84
C44	C33	C34	108.07	107.82	C46	C34	C33	107.94	108.31
C60	C34	C33	120.04	119.67	C60	C34	C46	119.76	120.23
C48	C35	C36	120.00	120.55	C60	C35	C36	108.11	107.67
C60	C35	C48	120.43	119.74	C37	C36	C35	108.01	108.24
C49	C36	C35	120.00	120.02	C49	C36	C37	120.33	119.74
C36	C37	C30	107.96	108.22	C38	C37	C30	119.96	120.03
C38	C37	C36	119.69	119.71	C37	C38	C28	119.93	120.64
C39	C38	C28	107.93	107.54	C39	C38	C37	119.71	119.76
C38	C39	C13	108.00	108.54	C40	C39	C13	120.04	120.30
C40	C39	C38	120.33	119.90	C39	C40	C31	120.07	120.59
C58	C40	C31	108.16	108.02	C58	C40	C39	120.15	119.45
C42	C41	C32	120.04	120.38	C58	C41	C32	107.83	107.93
C58	C41	C42	119.91	119.95	C43	C42	C41	119.89	119.83
C59	C42	C41	119.98	120.08	C59	C42	C43	107.85	108.15
C44	C43	C42	120.15	119.94	C57	C43	C42	107.89	107.58
C57	C43	C44	119.66	120.01	C43	C44	C33	119.80	120.26
C45	C44	C33	107.87	107.78	C45	C44	C43	120.04	119.81
C46	C45	C44	108.02	108.33	C55	C45	C44	120.13	120.27
C55	C45	C46	119.55	119.67	C45	C46	C34	108.09	107.75
C47	C46	C34	120.21	119.84	C47	C46	C45	120.18	120.24
C48	C47	C46	120.13	120.05	C53	C47	C46	120.27	119.78
C53	C47	C48	107.97	107.61	C47	C48	C35	119.61	120.26
C51	C48	C35	119.92	119.20	C51	C48	C47	107.92	108.14
C36	C49	C27	120.02	120.62	C50	C49	C27	108.07	107.57
C50	C49	C36	120.15	119.75	C49	C50	C25	108.04	108.52
C51	C50	C25	119.69	120.30	C51	C50	C49	119.74	119.95
C50	C51	C48	120.18	120.52	C52	C51	C48	108.20	108.13
C52	C51	C50	120.01	119.43	C51	C52	C23	120.32	120.53
C53	C52	C23	120.48	119.81	C53	C52	C51	107.75	107.59
C52	C53	C47	108.16	108.53	C54	C53	C47	119.55	120.37
C54	C53	C52	119.71	119.77	C53	C54	C21	119.95	120.48
C55	C54	C21	108.31	108.13	C55	C54	C53	120.26	119.39
C54	C55	C45	120.19	120.54	C56	C55	C45	119.77	119.79
C56	C55	C54	107.74	107.58	C55	C56	C20	108.03	108.54
C57	C56	C20	120.16	120.16	C57	C56	C55	120.18	120.03
C43	C57	C10	108.28	108.60	C56	C57	C10	119.95	119.69
C56	C57	C43	120.22	120.08	C40	C58	C29	119.59	120.41
C41	C58	C29	119.99	119.89	C41	C58	C40	108.03	108.00
C11	C59	C10	119.51	120.32	C42	C59	C10	108.14	108.08
C42	C59	C11	119.94	119.80	C34	C60	C30	119.84	120.46
C35	C60	C30	107.91	108.17	C35	C60	C34	119.87	119.87
RMSE = 0.39 °									

Table 11. Bond angles [°] comparison for $C_{60}(OH)_{24}$ as obtained by DFT and OPLS_2005

			DFT	OPLS_2005				DFT	OPLS_2005
C5	C1	C2	100.69	100.77	C9	C1	C2	110.28	112.03
C9	C1	C5	108.64	112.01	O61	C1	C2	115.21	110.70
O61	C1	C5	107.72	110.13	O61	C1	C9	113.33	110.82
C3	C2	C1	108.83	109.63	C12	C2	C1	123.19	122.43
C12	C2	C3	123.26	122.62	C4	C3	C2	100.21	100.65
C15	C3	C2	109.85	111.95	C15	C3	C4	108.55	112.40
O62	C3	C2	116.70	112.13	O62	C3	C4	113.16	109.12
O62	C3	C15	108.01	110.25	C5	C4	C3	112.57	112.70
C18	C4	C3	123.05	122.03	C18	C4	C5	123.42	123.24
C4	C5	C1	112.27	112.45	C6	C5	C1	122.76	122.28
C6	C5	C4	124.10	122.98	C7	C6	C5	108.96	112.30
C20	C6	C5	109.96	111.98	C20	C6	C7	100.20	100.63
O63	C6	C5	112.55	111.00	O63	C6	C7	113.21	110.04
O63	C6	C20	111.27	110.47	C8	C7	C6	122.74	121.91
C22	C7	C6	112.63	112.68	C22	C7	C8	123.58	123.26
C9	C8	C7	108.61	112.40	C25	C8	C7	110.26	111.97
C25	C8	C9	100.13	100.58	O64	C8	C7	108.32	110.19
O64	C8	C9	112.97	109.25	O64	C8	C25	116.20	112.13
C8	C9	C1	123.22	122.18	C10	C9	C1	123.58	123.18
C10	C9	C8	112.27	112.60	C11	C10	C9	123.97	123.05
C26	C10	C9	112.58	112.70	C26	C10	C11	122.70	122.25
C12	C11	C10	110.17	111.97	C29	C11	C10	108.68	112.04
C29	C11	C12	100.31	100.87	O65	C11	C10	107.32	109.78
O65	C11	C12	116.54	111.15	O65	C11	C29	113.56	110.79
C11	C12	C2	122.71	122.62	C13	C12	C2	123.04	122.69
C13	C12	C11	109.22	109.60	C14	C13	C12	109.75	111.97
C30	C13	C12	100.09	100.60	C30	C13	C14	108.55	112.50
O66	C13	C12	111.86	110.63	O66	C13	C14	113.42	110.82
O66	C13	C30	112.35	109.92	C15	C14	C13	124.16	123.13
C33	C14	C13	122.85	122.16	C33	C14	C15	112.18	112.43
C14	C15	C3	123.68	123.23	C16	C15	C3	122.83	122.04
C16	C15	C14	112.62	112.58	C17	C16	C15	108.80	112.41
C34	C16	C15	100.11	100.62	C34	C16	C17	109.76	111.99
O67	C16	C15	112.70	109.93	O67	C16	C17	113.78	111.22
O67	C16	C34	110.82	110.21	C18	C17	C16	122.95	122.16
C37	C17	C16	123.69	123.00	C37	C17	C18	112.15	112.45
C17	C18	C4	108.96	112.35	C19	C18	C4	109.95	111.89
C19	C18	C17	100.75	100.77	O68	C18	C4	113.11	110.78
O68	C18	C17	108.30	109.89	O68	C18	C19	114.91	110.80
C20	C19	C18	123.49	122.64	C38	C19	C18	108.70	109.64
C38	C19	C20	123.56	122.64	C19	C20	C6	122.82	122.63
C21	C20	C6	109.38	109.70	C21	C20	C19	122.72	122.65
C22	C21	C20	100.18	100.68	C40	C21	C20	109.82	111.94
C40	C21	C22	109.03	112.32	O69	C21	C20	117.16	111.31
O69	C21	C22	112.93	110.48	O69	C21	C40	107.44	109.85
C21	C22	C7	112.40	112.42	C23	C22	C7	123.92	122.94
C23	C22	C21	122.70	122.32	C24	C23	C22	110.10	112.00
C42	C23	C22	108.63	112.18	C42	C23	C24	100.18	100.71

O70	C23	C22	108.92	110.64	O70	C23	C24	116.12	110.91
O70	C23	C42	112.47	110.04	C25	C24	C23	123.00	122.74
C44	C24	C23	109.09	109.59	C44	C24	C25	123.38	122.79
C24	C25	C8	123.00	122.54	C26	C25	C8	109.11	109.77
C26	C25	C24	123.25	122.46	C25	C26	C10	100.19	100.46
C27	C26	C10	108.63	112.42	C27	C26	C25	109.81	112.12
O71	C26	C10	112.21	109.91	O71	C26	C25	111.54	110.47
O71	C26	C27	113.63	111.02	C28	C27	C26	122.60	121.97
C45	C27	C26	123.93	123.17	C45	C27	C28	112.57	112.55
C29	C28	C27	108.96	112.35	C47	C28	C27	100.19	100.76
C47	C28	C29	109.67	111.89	O72	C28	C27	112.39	109.72
O72	C28	C29	108.74	110.54	O72	C28	C47	116.50	111.24
C28	C29	C11	122.89	122.35	C30	C29	C11	112.34	112.30
C30	C29	C28	123.70	123.04	C29	C30	C13	112.74	112.80
C31	C30	C13	122.25	121.95	C31	C30	C29	124.27	123.20
C32	C31	C30	109.06	112.28	C48	C31	C30	109.82	111.89
C48	C31	C32	100.16	100.70	O73	C31	C30	107.45	109.87
O73	C31	C32	112.90	110.50	O73	C31	C48	117.17	111.33
C33	C32	C31	122.71	122.33	C50	C32	C31	112.43	112.41
C50	C32	C33	123.88	122.94	C32	C33	C14	108.60	112.21
C34	C33	C14	100.25	100.75	C34	C33	C32	110.08	112.03
O74	C33	C14	112.48	110.02	O74	C33	C32	108.96	110.61
O74	C33	C34	116.06	110.88	C33	C34	C16	108.99	109.59
C35	C34	C16	123.49	122.82	C35	C34	C33	123.10	122.73
C36	C35	C34	123.16	122.48	C51	C35	C34	122.89	122.50
C51	C35	C36	109.15	109.78	C37	C36	C35	109.82	112.10
C53	C36	C35	100.14	100.43	C53	C36	C37	108.63	112.38
O75	C36	C35	111.61	110.50	O75	C36	C37	113.58	111.05
O75	C36	C53	112.22	109.94	C36	C37	C17	123.98	123.17
C38	C37	C17	112.54	112.56	C38	C37	C36	122.58	121.96
C37	C38	C19	100.22	100.74	C39	C38	C19	109.64	111.93
C39	C38	C37	108.92	112.40	O76	C38	C19	116.54	111.22
O76	C38	C37	112.40	109.70	O76	C38	C39	108.74	110.51
C40	C39	C38	123.77	123.03	C54	C39	C38	122.90	122.34
C54	C39	C40	112.29	112.27	C39	C40	C21	124.23	123.19
C41	C40	C21	122.28	121.94	C41	C40	C39	112.76	112.79
C42	C41	C40	108.55	112.50	C55	C41	C40	100.10	100.65
C55	C41	C42	109.74	111.90	O77	C41	C40	112.32	109.93
O77	C41	C42	113.44	110.83	O77	C41	C55	111.86	110.63
C41	C42	C23	122.79	122.15	C43	C42	C23	112.20	112.49
C43	C42	C41	124.21	123.13	C44	C43	C42	112.68	112.54
C60	C43	C42	123.65	123.26	C60	C43	C44	122.81	122.05
C43	C44	C24	100.04	100.62	C45	C44	C24	109.82	112.04
C45	C44	C43	108.76	112.38	O78	C44	C24	110.86	110.21
O78	C44	C43	112.70	109.92	O78	C44	C45	113.79	111.22
C44	C45	C27	123.69	122.97	C46	C45	C27	112.12	112.46
C46	C45	C44	122.99	122.18	C47	C46	C45	100.75	100.75
C59	C46	C45	108.96	112.38	C59	C46	C47	109.98	111.93
O79	C46	C45	108.32	109.87	O79	C46	C47	114.86	110.77
O79	C46	C59	113.12	110.75	C46	C47	C28	108.73	109.64

C48	C47	C28	123.59	122.66	C48	C47	C46	123.45	122.63
C47	C48	C31	122.71	122.66	C49	C48	C31	109.37	109.69
C49	C48	C47	122.87	122.61	C50	C49	C48	100.20	100.61
C58	C49	C48	110.00	112.02	C58	C49	C50	108.95	112.34
O80	C49	C48	111.14	110.46	O80	C49	C50	113.14	110.02
O80	C49	C58	112.71	110.97	C49	C50	C32	112.59	112.69
C51	C50	C32	123.64	123.23	C51	C50	C49	122.76	121.93
C50	C51	C35	110.29	112.03	C52	C51	C35	100.14	100.53
C52	C51	C50	108.56	112.34	O81	C51	C35	116.22	112.14
O81	C51	C50	108.33	110.21	O81	C51	C52	112.94	109.26
C53	C52	C51	112.27	112.62	C57	C52	C51	123.22	122.21
C57	C52	C53	123.62	123.17	C52	C53	C36	112.62	112.71
C54	C53	C36	122.67	122.27	C54	C53	C52	123.95	123.06
C53	C54	C39	108.68	112.03	C55	C54	C39	100.34	100.91
C55	C54	C53	110.21	111.98	O82	C54	C39	113.51	110.77
O82	C54	C53	107.32	109.77	O82	C54	C55	116.53	111.14
C54	C55	C41	109.19	109.59	C56	C55	C41	123.04	122.78
C56	C55	C54	122.71	122.54	C57	C56	C55	123.19	122.49
C60	C56	C55	123.29	122.57	C60	C56	C57	108.87	109.62
C56	C57	C52	110.21	111.99	C58	C57	C52	108.67	112.00
C58	C57	C56	100.69	100.81	O83	C57	C52	113.30	110.83
O83	C57	C56	115.07	110.70	O83	C57	C58	107.95	110.12
C57	C58	C49	122.79	122.26	C59	C58	C49	124.03	122.98
C59	C58	C57	112.23	112.43	C58	C59	C46	123.44	123.23
C60	C59	C46	122.98	122.01	C60	C59	C58	112.62	112.69
C56	C60	C43	109.82	111.93	C59	C60	C43	108.63	112.43
C59	C60	C56	100.14	100.69	O84	C60	C43	108.00	110.23
O84	C60	C56	116.73	112.12	O84	C60	C59	113.15	109.11
H85	O61	C1	107.35	109.31	H86	O62	C3	107.03	108.92
H87	O63	C6	106.90	109.05	H88	O64	C8	106.82	108.68
H89	O65	C11	107.04	108.93	H90	O66	C13	106.64	108.52
H91	O67	C16	107.03	109.14	H92	O68	C18	107.24	109.27
H93	O69	C21	107.16	109.10	H94	O70	C23	106.53	108.93
H95	O71	C26	106.64	108.60	H96	O72	C28	106.58	108.97
H97	O73	C31	107.16	109.10	H98	O74	C33	106.53	108.93
H99	O75	C36	106.63	108.60	H100	O76	C38	106.59	108.98
H10	O77	C41	106.64	108.52	H102	O78	C44	107.02	109.14
H10	O79	C46	107.20	109.28	H104	O80	C49	106.92	109.05
H10	O81	C51	106.84	108.68	H106	O82	C54	107.05	108.93
H10	O83	C57	107.33	109.31	H108	O84	C60	107.03	108.92
RMSE = 2.13 °									