Supporting Information for "Applying Polymer Solubility Theory to Single Walled Carbon Nanotube Solutions"

Table S1 presents the molar volume values for the aryl carboxylic acid and aryl hydroxyl groups calculated from group additivity theory[1] as well as estimates for the bare carbon nanotube species under investigation[2].

Table S1. Summary of Molar Volume Calculations

CNT	d (nm)	#C/nm	V (nm^3)
(6,5)	0.76	89.5	953
(11,3)	1.01	119.8	1448
(10,10)	1.38	162.5	2321
R Groups			
C6H4-COOH	-	-	0.131
C6H4-OH	-	-	0.107

Table S2 shows the group additivity values used in the Refined Solubility Parameter and Fedors polymer solubility theories.

Table S2. Summary of Group Additivity Values

Data from *Van Krevelen, D.W., Properties of Polymers, Elsevier, New York, 1976*

Refined Solubility Parameter

	>C=	>C<	=CH-	-COOH	-OH	Ring
F_{di}	70	-70	200	530	210	1270
F_{pi}	0	0	0	420	500	110
E_{hi}	0	0	0	10000	20000	0

Fedors Method

Cohesive Energy (J/cm3)					
>C=	>C<	=CH-	-COOH	-OH	Ring
89518	0	0	0	0	0
93889	4370	17481	4370	0	4370
93889	4370	17481	0	4370	4370
119808	0	0	0	0	0
125657	5849	23396	5849	0	5849
125657	5849	23396	0	5849	5849
162537	0	0	0	0	0
170472	7935	31740	7935	0	7935
170472	7935	31740	0	7935	7935

Table S3 summarizes the solubility parameters (δ, SI units) and Flory-Huggins interaction parameters (χ) calculated for the OH-SWNT reaction series.

Table S3. Calculated Solubility Parameters and Flory-Huggins Interaction Parameter for OH-SWNT

		Refined Solubility Parameter			X - water			X - DMF		
Sample	**# FG / 100 C's**	**(6,5)**	**(11,3)**	**(10,10)**	**(6,5)**	**(11,3)**	**(10,10)**	**(6,5)**	**(11,3)**	**(10,10)**
P2	0.0	10.9	9.6	8.1	10.05	10.77	11.62	6.05	7.23	8.71
P2OH1	1.5	14.1	12.7	11.2	8.42	9.09	9.91	3.62	4.57	5.82
P2OH3	5.1	18.2	16.9	15.4	6.50	7.06	7.80	1.38	1.95	2.80
P2OH4	7.9	20.1	18.9	17.4	5.71	6.19	6.85	0.71	1.10	1.72
P2OH2	8.5	20.4	19.2	17.7	5.59	6.06	6.70	0.62	0.98	1.57

		Fedors			X - water			X - DMF		
Sample	**# FG / 100 C's**	**(6,5)**	**(11,3)**	**(10,10)**	**(6,5)**	**(11,3)**	**(10,10)**	**(6,5)**	**(11,3)**	**(10,10)**
P2	0.0	31.4	29.5	27.1	2.02	2.51	3.19	1.36	0.68	0.17
P2OH1	1.5	31.4	29.7	27.6	2.03	2.46	3.07	1.34	0.73	0.23
P2OH3	5.1	31.3	30.0	28.3	2.05	2.38	2.86	1.30	0.83	0.37
P2OH4	7.9	31.3	30.1	28.6	2.06	2.34	2.75	1.29	0.88	0.45
P2OH2	8.5	31.2	30.2	28.7	2.06	2.34	2.73	1.28	0.89	0.47

		Combined Maiti - Fedors			X - water			X - DMF		
Sample	**# FG / 100 C's**	**(6,5)**	**(11,3)**	**(10,10)**	**(6,5)**	**(11,3)**	**(10,10)**	**(6,5)**	**(11,3)**	**(10,10)**
P2	0.0	26.0	22.5	19.4	3.54	4.75	6.00	0.04	0.17	0.93
P2OH1	1.5	26.7	23.7	20.9	3.32	4.33	5.39	0.11	0.04	0.49
P2OH3	5.1	27.8	25.5	23.2	2.99	3.72	4.52	0.28	0.01	0.09
P2OH4	7.9	28.3	26.4	24.4	2.84	3.44	4.10	0.38	0.07	0.01
P2OH2	8.5	28.4	26.5	24.6	2.81	3.39	4.03	0.40	0.09	0.00

		Combined Maiti - RSP			X - water			X - DMF		
Sample	**# FG / 100 C's**	**(6,5)**	**(11,3)**	**(10,10)**	**(6,5)**	**(11,3)**	**(10,10)**	**(6,5)**	**(11,3)**	**(10,10)**
P2	0.0	26.0	22.5	19.4	3.54	4.75	6.00	0.04	0.17	0.93
P2OH1	1.5	29.8	26.0	22.4	2.44	3.56	4.79	0.76	0.04	0.18
P2OH3	5.1	35.3	31.3	27.4	1.18	2.06	3.13	3.44	1.29	0.20
P2OH4	7.9	38.1	34.0	29.9	0.73	1.45	2.39	5.48	2.60	0.82
P2OH2	8.5	38.5	34.4	30.4	0.66	1.36	2.28	5.86	2.86	0.96

Table S4 summarizes the solubility parameters (δ, SI units) and Flory-Huggins interaction parameters (χ) calculated for the OH-SWNT reaction series.

Table S4. Calculated Solubility Parameters and Flory-Huggins Interaction Parameter for COOH-SWNT

		Refined Solubility Parameter			X - water			X - DMF		
Sample	**# FG / 100 C's**	**(6,5)**	**(11,3)**	**(10,10)**	**(6,5)**	**(11,3)**	**(10,10)**	**(6,5)**	**(11,3)**	**(10,10)**
P2	0.0	10.9	9.6	8.1	10.05	10.77	11.62	6.05	7.23	8.71
P2COOH3	0.7	12.3	11.0	9.5	9.31	10.01	10.86	4.89	5.98	7.37
P2COOH2	1.0	12.8	11.4	9.9	9.09	9.78	10.62	4.56	5.61	6.98
P2COOH1	1.2	13.1	11.8	10.3	8.90	9.58	10.42	4.29	5.30	6.64
P2COOH4	1.6	13.6	12.3	10.8	8.64	9.31	10.14	3.91	4.88	6.18
P2COOH5	2.2	14.4	13.1	11.6	8.24	8.89	9.70	3.37	4.27	5.49
P2COOH6	3.0	15.3	14.0	12.4	7.84	8.46	9.25	2.86	3.67	4.80

		Fedors			X - water			X - DMF		
Sample	**# FG / 100 C's**	**(6,5)**	**(11,3)**	**(10,10)**	**(6,5)**	**(11,3)**	**(10,10)**	**(6,5)**	**(11,3)**	**(10,10)**
P2	0.0	31.4	29.5	27.1	2.02	2.51	3.19	1.36	0.68	0.17
P2COOH3	0.7	31.1	29.4	27.2	2.09	2.55	3.19	1.24	0.64	0.17
P2COOH2	1.0	31.0	29.3	27.2	2.12	2.56	3.19	1.20	0.63	0.17
P2COOH1	1.2	30.9	29.3	27.2	2.14	2.57	3.18	1.17	0.62	0.17
P2COOH4	1.6	30.8	29.2	27.2	2.17	2.59	3.18	1.12	0.60	0.17
P2COOH5	2.2	30.6	29.1	27.2	2.22	2.62	3.18	1.05	0.57	0.17
P2COOH6	3.0	30.4	29.0	27.2	2.27	2.64	3.17	0.98	0.55	0.18

		Combined Maiti - Fedors			X - water			X - DMF		
Sample	**# FG / 100 C's**	**(6,5)**	**(11,3)**	**(10,10)**	**(6,5)**	**(11,3)**	**(10,10)**	**(6,5)**	**(11,3)**	**(10,10)**
P2	0.0	26.0	22.5	19.4	3.54	4.75	6.00	0.04	0.17	0.93
P2COOH3	0.7	28.1	22.9	21.0	2.92	4.61	5.35	0.33	0.11	0.46
P2COOH2	1.0	28.7	23.1	21.5	2.73	4.56	5.14	0.47	0.10	0.35
P2COOH1	1.2	29.3	23.2	22.0	2.57	4.52	4.96	0.62	0.09	0.26
P2COOH4	1.6	26.3	23.3	20.6	3.47	4.46	5.51	0.06	0.07	0.56
P2COOH5	2.2	26.3	23.6	21.0	3.44	4.37	5.35	0.07	0.05	0.47
P2COOH6	3.0	26.4	23.8	21.4	3.41	4.28	5.19	0.08	0.03	0.37

		Combined Maiti - RSP			X - water			X - DMF		
Sample	**# FG / 100 C's**	**(6,5)**	**(11,3)**	**(10,10)**	**(6,5)**	**(11,3)**	**(10,10)**	**(6,5)**	**(11,3)**	**(10,10)**
P2	0.0	26.0	22.5	19.4	3.54	4.75	6.00	0.04	0.17	0.93
P2COOH3	0.7	26.1	24.4	20.0	3.50	4.09	5.75	0.05	0.01	0.74
P2COOH2	1.0	26.2	25.0	20.2	3.49	3.89	5.67	0.06	0.00	0.68
P2COOH1	1.2	26.2	25.5	20.3	3.48	3.71	5.60	0.06	0.01	0.63
P2COOH4	1.6	30.1	26.2	22.6	2.36	3.47	4.72	0.86	0.06	0.15
P2COOH5	2.2	31.3	27.4	23.7	2.04	3.12	4.33	1.32	0.20	0.04
P2COOH6	3.0	32.7	28.7	24.8	1.73	2.75	3.93	1.92	0.46	0.00

References:

(1) Ammon, H. L., Mitchell, S. *Propellants, Explosives, Pyrotechnics* **1998**, *23*, 260-265.

(2) Nair, N.; Kim, W. J.; Braatz, R. D.; Strano, M. S. *Langmuir* **2008**, *24*, 1790-1795.