

Supporting information for

## Hansen Solubility parameters for single walled carbon nanotube-solvent mixtures

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Calculation of Hansen parameters for selected solvents

Hansen parameters for the following solvents were not available in the literature.

DMPU (Dimethyl-tetrahydro-2-pyrimidinone), OPPN (3-(2-oxo-1-pyrrolidinyl)propanenitrile), N8P (N-Octylpyrrolidone), DMEU (dimethyl-imidazolidinone), NFP (N-formyl-piperidine), N12P (N-dodecyl-pyrrolidone).

Due to their high dispersibility, we felt it important to include them in this study. We calculated values for  $\delta_D$ ,  $\delta_P$  and  $\delta_H$  using the HSPiP software (<http://www.hansen-solubility.com/>). This software offers a number of algorithms to calculate solvent Hansen parameters. Two of these methods, the so-called Y-MB<sup>1</sup> method and the Stefanis-Panayiotou<sup>2</sup> method are particularly useful as they calculate the Hansen parameters based on the SMILES molecular structure of the solvent. We used both methods to calculate the Hansen parameters for all 14 solvents studied. We used the solvents with known Hansen parameters to test the outputs of the two calculations. We found that the Y-MB method gave the most accurate results for  $\delta_D$ . However, the Stefanis-Panayiotou method gave the most accurate results for  $\delta_H$ . In the case of  $\delta_P$ , neither method was particularly accurate but the average of the Y-MB and Stefanis-Panayiotou was generally reasonably close to the correct value. Thus for the solvents with unknown Hansen parameters, we took the Y-MB value of  $\delta_D$ , the average value of  $\delta_P$  and the Stefanis-Panayiotou value of  $\delta_H$ . These values are given in table 1.

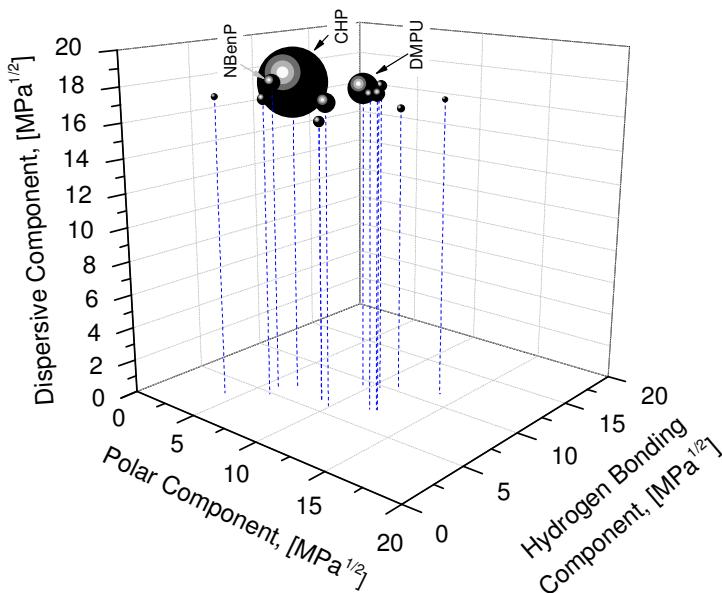


Figure S1: Position of the 14 best solvents studied in Hansen parameter space. The area of the data points is directly proportional to the nanotube dispersability in that solvent.

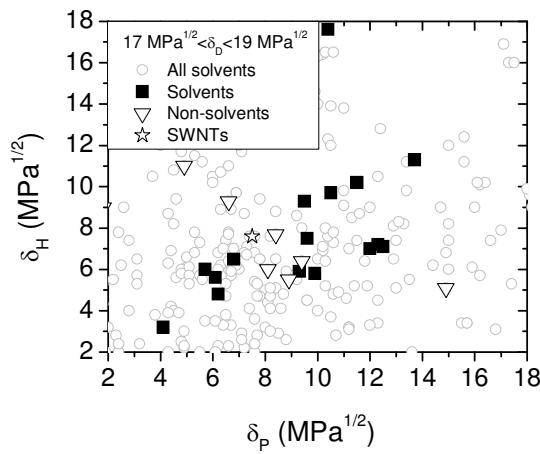


Figure S2: Relative position of solvents and non-solvents in the region of Hansen parameter space close to the nanotube solubility parameters ( $\delta_D=17.8$ ,  $\delta_P=7.5$ ,  $\delta_H=7.6$ , marked by star). Note this plot is a projection of all data with  $17 \text{ MPa}^{1/2} < \delta_D < 19 \text{ MPa}^{1/2}$ . Both solvents and non-solvents co-exist in the vicinity of the star. The gray circles represent all solvents from the HSPiP database with  $17 \text{ MPa}^{1/2} < \delta_D < 19 \text{ MPa}^{1/2}$ .

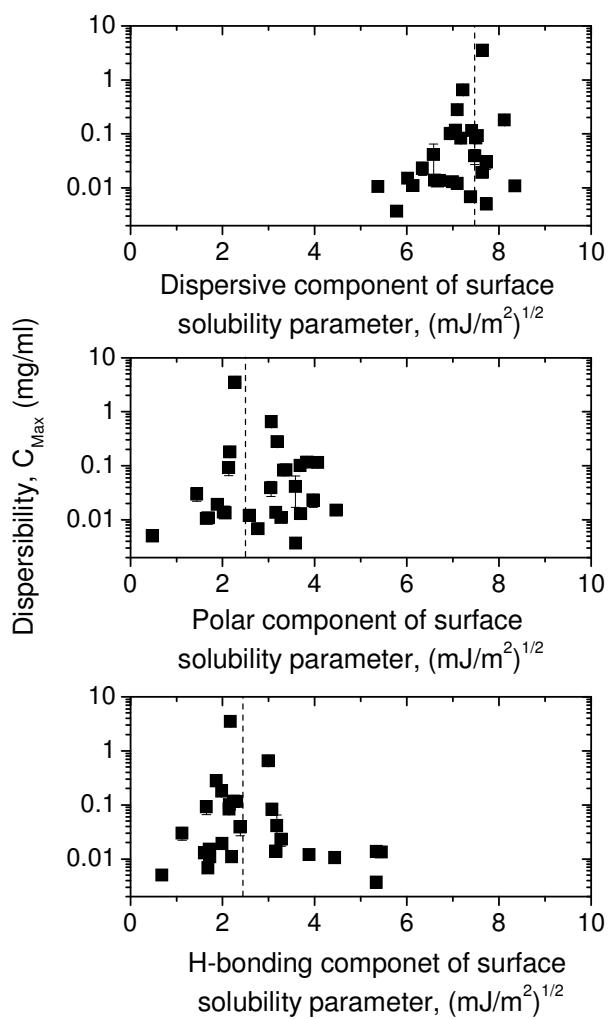


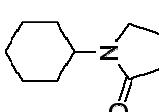
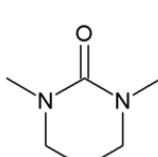
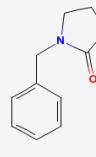
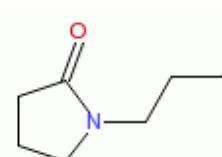
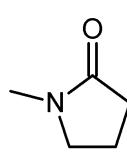
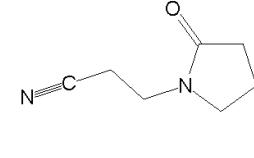
Figure S3: Dispersibility versus proposed surface energy solubility parameters,  $\delta_D$ ,  $\delta_P$  and  $\delta_H$ .

Solvent	$\delta_D$ (MPa $^{1/2}$ )	$\delta_P$ (MPa $^{1/2}$ )	$\delta_H$ (MPa $^{1/2}$ )	$C_{\text{Max}}$ (mg/ml)
CHP	18.2	6.8	6.5	3.5
DMPU	17.8	9.5	9.3	0.65
NBP	17.5	9.9	5.8	0.279
NBenzyl P	18.2	6.1	5.6	0.18
NMP	18	12.3	7.2	0.116
OPPN	18.1	12.5	7.1	0.115
NEP	18	12	7	0.101
N8P	17.4	6.2	4.8	0.092
NVP	16.4	9.3	5.9	0.084
DMEU	18	10.5	9.7	0.083
DMA	16.8	11.5	10.2	0.041
NFP	18.7	9.6	7.5	0.039

N12P	17.5	4.1	3.2	0.03
DMF	17.4	13.7	11.3	0.023
Benzyl acetate	18.3	5.7	6	0.0192
propionitrile	15.3	14.3	5.5	0.015
Acrylic acid	16.6	6.4	10	0.0138
2,2'-thiodiethanol	17.6	10.4	17.6	0.0136
Ethanol amine	17.5	6.8	18	0.0133
Cyclopentanone	17.9	11.9	5.2	0.0129
Chlorophenol	19.2	8.8	13.2	0.012
Acetone	15.5	10.4	7	0.011
Benzyl benzoate	20	5.1	5.2	0.0109
IPA	15.8	6.1	16.4	0.0105
Cyclohexanone	17.8	8.4	5.1	0.0068
Toluene	18	1.4	2	0.005
Triethyleneglycol	16	12.5	18.6	0.0037
Formamide	17.2	26.2	19	3E-4
Benzyl alcohol	18.4	6.3	13.7	2.79E-4
Nitropropane	16.6	12.3	5.5	0
ethylene glycol	16.8	15.8	27.7	0
tetraethylene glycol	16.7	12.9	19.6	0
Triethylenephosphate	16.7	11.4	9.2	0
diethylenetriamine	16.7	7.1	14.3	0
Diethylenetriamine	16.7	7.1	14.3	0
THF	16.8	5.7	8	0
formamide	26.2	19	17.2	0
2-Methoxy-1,3-Dioxolane	17.8	8.4	7.7	0
2-pyrrolidone	17.4	11.3	19.4	0
acrylonitrile	17.4	6.8	16.4	0
Dichloroacetonitrile	17.4	9.4	6.4	0
Pulegone	17.5	8.9	5.5	0
dibenzyl ether	19.6	3.4	5.2	0
Dioxane	17.5	1.8	9	0
benzophenone	19.5	7.2	5.1	0
Dioxolane	18.1	6.6	9.3	0
Benzaldehyde	19.4	7.4	5.3	0
morpholine	18	4.9	11	0
Diethyleneglycol	16.6	12	19	0
1,3-Butanediol	16.5	8.1	20.9	0
1,1-dichloroethane	16.5	7.8	3	0
Dimethylsulphate	16.5	13	7	0
Ethyl-Chloroformate	16.4	11	8	0
2-nitropropane	16.2	12.1	4.1	0
Acrylonitrile	16	12.8	6.8	0
dichloromethane	18.2	6.1	18.2	0
Bromotrichloromethane	18.3	8.1	6	0
furfural	18.6	14.9	5.1	0
Heptane	15.3	0	0	0
Hexofluoroctane	15.3	0	0	0
Hexofluorohexane	15.3	0	0	0
Aniline	20.1	5.8	11.2	0

Acetonitrile	15.3	18	6.1	0
Tert-butylchloride	15.1	9.4	3	0

Table S1 Solvent data for all solvents studied

Solvent	SMILES	Structure	$\delta_D$ (MPa <sup>1/2</sup> )	$\delta_P$ (MPa <sup>1/2</sup> )	$\delta_H$ (MPa <sup>1/2</sup> )
CHP <sup>A</sup> (Cyclohexyl-pyrrolidinone)	C1CCC(CC1)N2		<b>18.2</b>	<b>6.8</b>	<b>6.5</b>
	CCCC2=O		18.1	7.4	6
			16.8	6.5	6.1
			17.45	6.95	6.05
DMPU (Dimethyl-tetrahydro-2-pyrimidinone)	O=C1N(C)CCCN1C		17.8	12	9.3
			16.4	6.9	9.3
			17.8	9.5	9.3
NBenP (Benzyl-pyrrolidinone)	C1CC(=O)N(C1)CC2=CC=CC=C2		<b>18.2</b>	<b>6.1</b>	<b>5.6</b>
			19.5	6.7	6
			17.8	5.4	6.2
			18.65	6.05	6.1
NBP (N-butyl-Pyrrolidinone)	CCCCN1CCCC1=O		<b>17.5</b>	<b>9.9</b>	<b>5.8</b>
			17.4	9.7	5.1
			15.2	4.9	6.3
			16.3	7.3	5.7
NMP (N-methyl-pyrrolidinone)	CN1CCCC1=O		<b>18</b>	<b>12.3</b>	<b>7.2</b>
			17.7	13.9	7.8
			15.2	5.8	7.5
			16.45	9.35	7.65
OPPN(3-(2-oxo-1-pyrrolidinyl)propenenitrile)	O=C1CCCN1CC#N		18.1	11.5	8.1
			16.0	13.5	7.1
			18.1	12.5	7.1

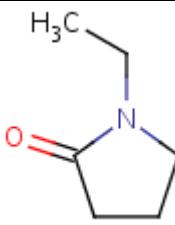
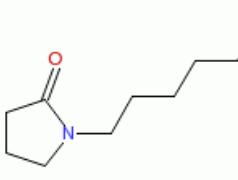
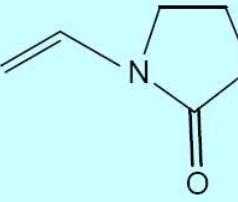
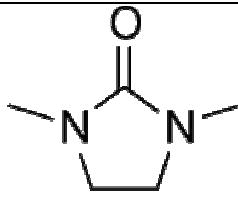
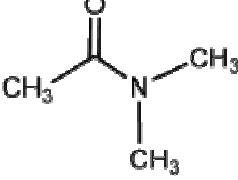
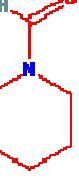
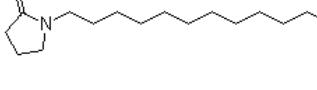
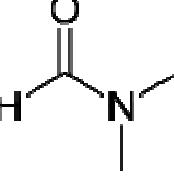
NEP (N-ethyl-Pyrrolidinone)	CCN1CCCC1=O		<b>18</b> 17.2 15.2 16.2	<b>12</b> 12.5 5.5 9	<b>7</b> 7.2 7.1 7.15
N8P (N-Octyl-pyrrolidone)	CCCCCCCN1C CCC1=O		17.4 15.3 17.4	8.8 3.6 6.2	4.3 4.8 4.8
NVP (N-vinyl-Pyrrolidinone)	N1(C(CC1)=O) C=C		<b>16.4</b> 17.4 15.2 16.3	<b>9.3</b> 11.8 5.4 8.6	<b>5.9</b> 8 7.1 7.55
DMEU (dimethyl-imidazolidinone)	CN1CCN (C1=O) C		18.0 16.4 18.0	13.6 7.2 10.5	10.2 9.7 9.7
DMA (dimethylacetamide)	O=C (C) N (C) C		<b>16.8</b> 17.4 16.8 17.1	<b>11.5</b> 14.6 11.5 13	<b>10.2</b> 10.3 10.2 10.25
NFP (N-formyl-piperidine)	O=CN1CCCCC1		18.7 16.1 18.7	12.4 6.8 9.6	8.3 7.5 7.5
N12P (N-dodecyl-pyrrolidone)	CCCCCCCCCCCCN 1CCCC1=O		17.5 15.3 17.5	5.8 2.3 4.1	3.6 3.2 3.2
DMF (dimethylformamide)	O=CN (C) C		<b>17.4</b> 17.7 14.2 15.9	<b>13.7</b> 17.2 5.1 11.1	<b>11.3</b> 11.5 7.9 9.7

Table S2 Detailed solvent information for the best 14 solvents. Bold values are measured D,P,H,  
Normal font represents calculated values. Normal font, top line: Y-MB, middle line: S-P, Bottom  
line: means of Y-MB and S-P

1. Isu, Y.; Nagashima, U.; Aoyama, T.; Hosoya, H., Development of neural network simulator for structure-activity correlation of molecules (NECO). Prediction of endo/exo substitution of norbornane derivatives and of carcinogenic activity of PAHs from C-13-NMR shifts. *Journal of Chemical Information and Computer Sciences* **1996**, 36, (2), 286-293.
2. Stefanis, E.; Panayiotou, C., Prediction of Hansen solubility parameters with a new group-contribution method. *International Journal of Thermophysics* **2008**, 29, (2), 568-585.