Theoretical Prediction of the Solubility of Fluorinated C_{60}

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Supplementary Material

Table S1 Results for the calculated solubilities (log $x_{2,calc}$) using equation 5. Values are tabulated according to increasing value for log $x_{2,exp}$, as taken from reference [16], with adapted values due to the forming of solvated crystals underlined (see text). Values for log x_2 lower than (-4,34 ± 0,43) printed in green indicate solubilities above the "ideal" solubility threshold.

Solvent	log $x_{2,exp}$	log $x_{2,calc}$
Chlorobenzene	-2.991	-3.267
Benzene	-3.161	-3.176
Toluene	-3.377	-3.301
Tetrachloromethane	-3.420	-3.773
Aniline	-3.875	-3.736
Dichloromethane	-4.699	-4.580
Trichloromethane	-4.745	-4.403
n-Heptane	-4.921	-4.728
1,2-Dichloroethane	-5.046	-5.106
Tetrahydrofurane	-5.155	-5.200
Cyclohexane	-5.268	-5.313
Ethanol	-7.086	-7.651
Methanol	-8.699	-8.320
Dimethylsulfoxide	-	-12.510
Water	-	-16.879

Table S2 Electrostatic (ΔE_{es}), cavity (ΔE_{cav}), dispersion (ΔE_{disp}), repulsion (ΔE_{rep}) and total energy difference (ΔE_{tot}) between the solvent and the gas phase for $C_{60}F_2$ in kcal/mol.

Solvent	ΔE_{es}	ΔE_{cav}	ΔE_{disp}	ΔE_{rep}	ΔE_{tot}
Water	**-12.54**	**47.32**	**-42.44**	**2.43**	**-5.23**
Dimethylsulfoxide	**-7.74**	**44.65**	**-44.28**	**2.52**	**-4.85**
Methanol	**-4.29**	**34.08**	**-36.74**	**2.04**	**-4.91**
Ethanol	**-3.82**	**34.70**	**-37.64**	**2.06**	**-4.70**
Dichloromethane	**-4.26**	**34.83**	**-36.71**	**2.06**	**-4.08**
Tetrahydrofurane	**-6.83**	**40.92**	**-40.12**	**2.18**	**-3.85**
Chlorobenzene	**-6.52**	**40.89**	**-41.31**	**3.46**	**-3.48**
Toluene	**-1.67**	**37.46**	**-41.46**	**3.59**	**-2.08**
Benzene	**-3.02**	**38.12**	**-40.67**	**3.58**	**-1.99**

Table S3 Electrostatic (ΔE_{es}), cavity (ΔE_{cav}), dispersion (ΔE_{disp}), repulsion (ΔE_{rep}) and total energy difference (ΔE_{tot}) between the solvent and the gas phase for $C_{60}F_4$ in kcal/mol.

Solvent	ΔE_{es}	ΔE_{cav}	ΔE_{disp}	ΔE_{rep}	ΔE_{tot}
Water	**-15.51**	**48.84**	**-43.38**	**2.49**	**-7.56**
Dimethylsulfoxide	**-10.46**	**46.14**	**-45.23**	**2.57**	**-6.98**
Methanol	**-6.74**	**35.21**	**-37.56**	**2.09**	**-7.00**
Ethanol	**-6.25**	**35.86**	**-38.48**	**2.11**	**-6.76**
Dichloromethane	**-6.50**	**36.00**	**-37.43**	**2.08**	**-5.85**
Tetrahydrofurane	**-9.09**	**42.29**	**-41.01**	**2.23**	**-5.58**
Chlorobenzene	**-8.64**	**42.27**	**-42.16**	**3.52**	**-5.01**
Toluene	**-3.01**	**38.73**	**-42.34**	**3.66**	**-2.96**
Benzene	**-4.33**	**39.41**	**-41.54**	**3.65**	**-2.81**

Table S4 Electrostatic (ΔE_{es}), cavity (ΔE_{cav}), dispersion (ΔE_{disp}), repulsion (ΔE_{rep}) and total energy difference (ΔE_{tot}) between the solvent and the gas phase for $C_{60}F_6$ in kcal/mol.

Solvent	ΔE_{es}	ΔE_{cav}	ΔE_{disp}	ΔE_{rep}	ΔE_{tot}
Water	**-19.01**	**50.93**	**-44.09**	**2.53**	**-9.64**
Dimethylsulfoxide	**-13.90**	**48.16**	**-45.89**	**2.59**	**-9.04**
Methanol	**-9.82**	**36.75**	**-38.14**	**2.11**	**-9.10**
Ethanol	**-9.29**	**37.44**	**-39.07**	**2.14**	**-8.78**
Dichloromethane	**-9.25**	**37.59**	**-38.02**	**2.10**	**-7.58**
Tetrahydrofurane	**-11.98**	**44.16**	**-41.62**	**2.25**	**-7.19**
Chlorobenzene	**-11.36**	**44.14**	**-42.87**	**3.57**	**-6.52**
Toluene	**-4.97**	**40.46**	**-43.06**	**3.71**	**-3.86**
Benzene	**-6.28**	**41.16**	**-42.24**	**3.70**	**-3.66**

Table S5 Electrostatic (ΔE_{es}), cavity (ΔE_{cav}), dispersion (ΔE_{disp}), repulsion (ΔE_{rep}) and total energy difference (ΔE_{tot}) between the solvent and the gas phase for $C_{60}F_8$ in kcal/mol.

Solvent	ΔE_{es}	ΔE_{cav}	ΔE_{disp}	ΔE_{rep}	ΔE_{tot}
Water	**-22.50**	**53.08**	**-44.93**	**2.59**	**-11.76**
Dimethylsulfoxide	**-17.10**	**50.25**	**-46.72**	**2.63**	**-10.94**
Methanol	**-12.67**	**38.34**	**-38.86**	**2.16**	**-11.03**
Ethanol	**-12.09**	**39.07**	**-39.80**	**2.18**	**-10.64**
Dichloromethane	**-11.91**	**39.23**	**-38.67**	**2.12**	**-9.23**
Tetrahydrofurane	**-14.73**	**46.08**	**-42.39**	**2.29**	**-8.75**
Chlorobenzene	**-13.95**	**46.07**	**-43.65**	**3.63**	**-7.90**
Toluene	**-6.83**	**42.23**	**-43.86**	**3.78**	**-4.68**
Benzene	**-8.14**	**42.96**	**-43.03**	**3.77**	**-4.44**

Table S6 Electrostatic (ΔE_{es}), cavity (ΔE_{cav}), dispersion (ΔE_{disp}), repulsion (ΔE_{rep}) and total energy difference (ΔE_{tot}) between the solvent and the gas phase for $C_{60}F_{10}$ in kcal/mol.

Solvent	ΔE_{es}	ΔE_{cav}	ΔE_{disp}	ΔE_{rep}	ΔE_{tot}
Water	**-25.63**	**55.23**	**-45.78**	**2.64**	**-13.54**
Dimethylsulfoxide	**-20.05**	**52.34**	**-47.55**	**2.67**	**-12.59**
Methanol	**-15.23**	**39.93**	**-39.58**	**2.20**	**-12.68**
Ethanol	**-14.71**	**40.70**	**-40.53**	**2.22**	**-12.32**
Dichloromethane	**-14.32**	**40.87**	**-39.32**	**2.15**	**-10.62**
Tetrahydrofurane	**-17.21**	**48.01**	**-43.16**	**2.33**	**-10.03**
Chlorobenzene	**-16.33**	**48.01**	**-44.43**	**3.69**	**-9.06**
Toluene	**-8.48**	**44.01**	**-44.67**	**3.85**	**-5.29**
Benzene	**-9.79**	**44.76**	**-43.82**	**3.83**	**-5.02**

Table S7 Electrostatic (ΔE_{es}), cavity (ΔE_{cav}), dispersion (ΔE_{disp}), repulsion (ΔE_{rep}) and total energy difference (ΔE_{tot}) between the solvent and the gas phase for $C_{60}F_{12}$ in kcal/mol.

Solvent	ΔE_{es}	ΔE_{cav}	ΔE_{disp}	ΔE_{rep}	ΔE_{tot}
Water	**-28.75**	**57.41**	**-46.62**	**2.69**	**-15.27**
Dimethylsulfoxide	**-22.87**	**54.44**	**-48.53**	**2.73**	**-14.23**
Methanol	**-17.79**	**41.53**	**-40.30**	**2.24**	**-14.32**
Ethanol	**-17.23**	**42.35**	**-41.26**	**2.26**	**-13.88**
Dichloromethane	**-16.36**	**42.52**	**-40.25**	**2.19**	**-11.90**
Tetrahydrofurane	**-19.65**	**49.95**	**-43.93**	**2.38**	**-11.25**
Chlorobenzene	**-18.56**	**49.95**	**-45.31**	**3.76**	**-10.16**
Toluene	**-10.15**	**45.80**	**-45.49**	**3.92**	**-5.92**
Benzene	**-11.46**	**46.57**	**-44.62**	**3.90**	**-5.61**

Table S8 Electrostatic (ΔE_{es}), cavity (ΔE_{cav}), dispersion (ΔE_{disp}), repulsion (ΔE_{rep}) and total energy difference (ΔE_{tot}) between the solvent and the gas phase for $C_{60}F_{14}$ in kcal/mol.

Solvent	ΔE_{es}	ΔE_{cav}	ΔE_{disp}	ΔE_{rep}	ΔE_{tot}
Water	**-32.10**	**59.55**	**-47.44**	**2.74**	**-17.25**
Dimethylsulfoxide	**-26.00**	**56.52**	**-49.18**	**2.75**	**-15.91**
Methanol	**-20.46**	**43.11**	**-40.99**	**2.28**	**-16.06**
Ethanol	**-19.74**	**43.96**	**-41.97**	**2.30**	**-15.45**
Dichloromethane	**-19.03**	**44.14**	**-40.61**	**2.19**	**-13.31**
Tetrahydrofurane	**-22.18**	**51.86**	**-44.67**	**2.41**	**-12.58**
Chlorobenzene	**-21.05**	**51.87**	**-45.98**	**3.80**	**-11.36**
Toluene	**-11.91**	**47.56**	**-46.27**	**3.98**	**-6.64**
Benzene	**-13.25**	**48.36**	**-45.38**	**3.96**	**-6.31**

Table S9 Electrostatic (ΔE_{es}), cavity (ΔE_{cav}), dispersion (ΔE_{disp}), repulsion (ΔE_{rep}) and total energy difference (ΔE_{tot}) between the solvent and the gas phase for $C_{60}F_{16}$ in kcal/mol.

Solvent	ΔE_{es}	ΔE_{cav}	ΔE_{disp}	ΔE_{rep}	ΔE_{tot}
Water	**-35.09**	**61.82**	**-48.38**	**2.81**	**-18.84**
Dimethylsulfoxide	**-28.83**	**58.72**	**-50.03**	**2.79**	**-17.35**
Methanol	**-22.91**	**44.78**	**-41.76**	**2.33**	**-17.56**
Ethanol	**-22.23**	**45.68**	**-42.74**	**2.35**	**-16.94**
Dichloromethane	**-21.32**	**45.87**	**-41.25**	**2.22**	**-14.48**
Tetrahydrofurane	**-24.62**	**53.89**	**-45.46**	**2.46**	**-13.73**
Chlorobenzene	**-23.30**	**53.91**	**-46.86**	**3.88**	**-12.37**
Toluene	**-13.51**	**49.44**	**-47.19**	**4.06**	**-7.20**
Benzene	**-14.87**	**50.26**	**-46.29**	**4.05**	**-6.85**

Table S10 Electrostatic (ΔE_{es}), cavity (ΔE_{cav}), dispersion (ΔE_{disp}), repulsion (ΔE_{rep}) and total energy difference (ΔE_{tot}) between the solvent and the gas phase for $C_{60}F_{18}$ in kcal/mol.

Solvent	ΔE_{es}	ΔE_{cav}	ΔE_{disp}	ΔE_{rep}	ΔE_{tot}
Water	**-42.58**	**68.73**	**-49.11**	**2.86**	**-20.10**
Dimethylsulfoxide	**-35.71**	**65.28**	**-50.80**	**2.84**	**-18.39**
Methanol	**-28.53**	**49.79**	**-42.41**	**2.37**	**-18.78**
Ethanol	**-27.72**	**50.79**	**-43.42**	**2.39**	**-17.96**
Dichloromethane	**-26.69**	**51.00**	**-41.86**	**2.24**	**-15.31**
Tetrahydrofurane	**-30.76**	**59.91**	**-46.19**	**2.50**	**-14.54**
Chlorobenzene	**-29.39**	**59.94**	**-47.50**	**3.92**	**-13.03**
Toluene	**-18.73**	**54.97**	**-47.86**	**4.11**	**-7.51**
Benzene	**-20.15**	**55.88**	**-46.93**	**4.10**	**-7.10**

Table S11 Electrostatic (ΔE_{es}), cavity (ΔE_{cav}), dispersion (ΔE_{disp}), repulsion (ΔE_{rep}) and total energy difference (ΔE_{tot}) between the solvent and the gas phase for $C_{60}F_{20}$ in kcal/mol.

Solvent	ΔE_{es}	ΔE_{cav}	ΔE_{disp}	ΔE_{rep}	ΔE_{tot}
Water	**-40.70**	**66.46**	**-50.20**	**2.91**	**-21.53**
Dimethylsulfoxide	**-33.88**	**63.20**	**-51.88**	**2.89**	**-19.67**
Methanol	**-27.32**	**48.19**	**-43.40**	**2.42**	**-20.11**
Ethanol	**-26.38**	**49.18**	**-44.44**	**2.44**	**-19.20**
Dichloromethane	**-25.33**	**49.39**	**-42.66**	**2.27**	**-16.33**
Tetrahydrofurane	**-28.77**	**58.01**	**-47.25**	**2.55**	**-15.46**
Chlorobenzene	**-27.59**	**58.05**	**-48.37**	**3.97**	**-13.94**
Toluene	**-16.65**	**53.24**	**-48.8**	**4.17**	**-8.04**
Benzene	**-18.03**	**54.12**	**-47.83**	**4.15**	**-7.59**

Table S12 Cavity volume for $C_{60}F_{2n}$ with n = 1-10, calculated within the PCM formalism.

Solvent	$C_{60}F_2$	$C_{60}F_4$	$C_{60}F_6$	$C_{60}F_8$	$C_{60}F_{10}$	$C_{60}F_{12}$	$C_{60}F_{14}$	$C_{60}F_{16}$	$C_{60}F_{18}$	$C_{60}F_{20}$
Chlorobenzene	380.44	394.17	407.27	420.76	433.71	447.91	461.53	474.74	490.20	501.09
Benzene	381.98	393.92	406.82	420.30	433.17	447.49	460.72	473.82	489.19	500.69
Toluene	380.49	393.78	407.26	420.82	433.57	447.81	461.49	474.82	490.19	501.14
Dichloromethane	381.25	393.01	405.96	419.23	432.25	445.66	459.74	473.27	487.27	499.78
Tetrahydrofurane	382.88	393.14	406.70	420.11	433.03	447.04	460.93	473.74	488.82	500.50
Ethanol	381.87	392.79	405.73	419.37	431.91	445.34	459.39	472.00	486.31	499.32
Methanol	380.80	392.24	405.20	418.16	431.37	444.38	457.54	470.34	485.30	495.46
Dimethylsulfoxide	379.73	394.49	406.29	419.83	432.92	446.51	459.99	473.45	488.24	500.05
Water	380.37	390.96	403.81	416.31	429.15	442.48	454.79	467.61	481.35	493.06

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