

Supplementary Material

Unravelling donor-acceptor film morphology formation for environmentally-friendly OPV ink formulations

Natalie P. Holmes^{a,b*}, Holly Munday^b, Matthew G. Barr^b, Lars Thomsen^c, Matthew A. Marcus^d, A. L. David Kilcoyne^d, Adam Fahy^b, Jan van Stam^e, Paul C. Dastoor^b, Ellen Moons^a

^a Department of Engineering and Physics, Karlstad University, Karlstad 65188, Sweden

^b Centre for Organic Electronics, University of Newcastle, Callaghan NSW 2308, Australia

^c Australian Synchrotron, ANSTO, Clayton, VIC 3168, Australia

^d Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

^e Department of Engineering and Chemical Sciences, Karlstad University, 65188 Karlstad, Sweden

*Corresponding author: Natalie P. Holmes, natalie.holmes@newcastle.edu.au

1. List of solvents utilised for solubility tests

Table S1. Solvents utilised for solubility tests, with good solvents and non-solvents identified.

Solvent	Solubility Identification	
	TQ1	PC ₆₁ BM
Acetone	Non-solvent	Non-solvent
1-Butanol	Non-solvent	Non-solvent
2-Butanol	Non-solvent	Non-solvent
Butyl acetate	Non-solvent	Good solvent
Chlorobenzene	Good solvent	Good solvent
Chloroform	Good solvent	Good solvent
Cyclohexane	Non-solvent	Non-solvent
Cyclohexanone	Good solvent	Good solvent
Cyclopentyl methyl ether	Good solvent	Good solvent
Dichloromethane	Good solvent	Good solvent
Dimethyl sulfoxide	Non-solvent	Non-solvent
Dipropyl amine	Good solvent	Non-solvent
Dipropylene glycol	Non-solvent	Non-solvent
Ethanol	Non-solvent	Non-solvent
Ethyl acetate	Non-solvent	Non-solvent
Ethyl benzene	Good solvent	Good solvent
Formamide	Non-solvent	Non-solvent
Glycerol	Non-solvent	Non-solvent
Isopropyl acetate	Non-solvent	Non-solvent
Isopropyl benzene	Good solvent	Good solvent
Mesitylene	Good solvent	Good solvent
Methylacetate	Non-solvent	Non-solvent
Methyl cyclohexane	Non-solvent	Non-solvent
2-Methyl tetrahydrofuran	Good solvent	Good solvent
N-Methyl formamide	Non-solvent	Non-solvent
N,N-Dimethylformamide	Non-solvent	Non-solvent
1-Octanol	Non-solvent	Non-solvent
o-Dichlorobenzene	Good solvent	Good solvent
Pentyl acetate	Non-solvent	Good solvent
2-Propanol	Non-solvent	Non-solvent
Propylene carbonate	Non-solvent	Non-solvent
Tetrahydronaphthalene	Good solvent	Good solvent
Tetrahydrofuran	Good solvent	Good solvent
Toluene	Good solvent	Good solvent
o-Xylene	Good solvent	Good solvent
Water	Non-solvent	Non-solvent

A disadvantage of the HSP method is that a large amount of material is required for the numerous solubility tests to generate data for the HSP calculation. Rather than choosing a concentration of 15 - 30 mg ml⁻¹ for the initial solubility tests we chose a concentration of 1 mg ml⁻¹ to minimise material use.

2. BHJ film preparation

Table S2. Spin coating and drying conditions for BHJ films. Thermal drying was utilised to remove residual solvent and additive.

Ink Code	TQ1:PC₆₁BM w/w Ratio	Spin Coating Speed (RPM)	Spin Coating Time (min)	Drying Temperature (°C)	Drying Time (min)
Lim	1:2	2000	1	80	10
Lim:2-MA	1:2	2000	1	80	10
Lim:MO	1:2	2000	1	80	10
Lim:MY	1:2	2000	1	80	10
Ani:DE	1:2	2000	1	140	5
Ani:DIO	1:2	1300	1	100	5
2-MA:Lim	1:2	2000	1	140	5
o-DCB (Ref)	1:1	2000	1	80	10

3. Safety phrases and classification of solvents and additives

Table S3. Toxicity, biodegradability and hazard statements for solvents and additives.

Solvent/Additive	Oral Toxicity (LD₅₀) mg/kg	Hazard Code	Biodegradability
d-Limonene	>5000; 4400	H226, H304, H315, H317, H410	71 % - Readily biodegradable (OECD Test Guideline 301B - CO ₂ evolution)
2-Methylanisole	>2000	H226, H315	Low persistence in air and soil. Low bioaccumulative potential.
Anisole	3700	H226	Biodegradable
Diphenyl ether	3370	H410	62% Ratio BOD/ThBOD*
1- Methylnaphthalene	1840	H302, H315, H317, H319, H410	Not readily biodegradable
1- Methoxynaphthalene	Information not available	H317, H410	High persistence in water/soil and air. Low bioaccumulative potential.
o-Dichlorobenzene	500	H302, H332, H315, H317, H319, H335, H410	Not readily biodegradable
1,8-Diiodooctane	Information not available	H302, H315, H319, H335	High persistence in water/soil and air. High bioaccumulative potential.

*ThOD = Theoretical oxygen demand

BOD = Biochemical oxygen demand

H226: Flammable liquid and vapor [Warning: flammable liquids].

H302: Harmful if swallowed.

H304: May be fatal if swallowed and enters airways [Danger: aspiration hazard].

H315: Causes skin irritation [Warning: skin corrosion/irritation].

H317: May cause an allergic skin reaction [Warning: sensitisation, skin].

H319: Causes serious eye irritation [Warning: serious eye damage/eye irritation].

H332: Harmful if inhaled [Warning: acute toxicity, inhalation].

H335: May cause respiratory irritation [Warning: specific target organ toxicity, single exposure; respiratory tract irritation].

H336: May cause drowsiness or dizziness [Warning: specific target organ toxicity, single exposure; narcotic effects].

H373: Causes damage to organs through prolonged or repeated exposure [Warning: specific target organ toxicity, repeated exposure].

H400: Very toxic to aquatic life [Warning: hazardous to the aquatic environment, acute hazard].

H410: Very toxic to aquatic life with long lasting effects [Warning: hazardous to the aquatic environment, long-term hazard].