Electronic Supplementary Material (ESI) for Green Chemistry.

Environmental, Cost, and Chemical Hazards of Using Alternative Green Solvents for Fullerene (C_{60}) Purification

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Content: 10 figures and five tables (7 pages)

S1 – C_{60} production process

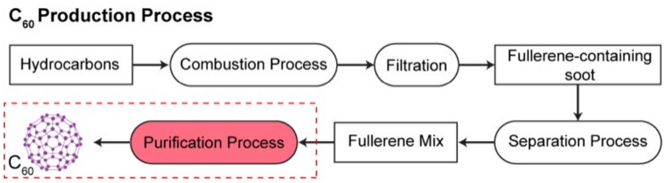

Fig. S1. C_{60} synthesis procedure – Rectangulars show materials. Red dashed lines demonstrate the study scope of this study, and C_{60} purification is distinguished in the red box.

S2 – Green chemistry principles

Table S1. Green chemistry principles (1)

Principle #	Description	How we used
1	Waste prevention instead of cleaning waste after it is formed	N/A
2	Maximize the incorporation of all used materials into the final products	N/A
3	Using substances that have little or no toxicity for human health and the environment	We categorized potential solvents based on toxicity scores and identified alternative solvents with lower toxicity.
4	Design safer chemicals with lower environmental toxicity	We identified non-hazardous alternative solvents to avoid toxifying the final products.
5	Use less solvents	We categorized potential solvents based on their fullerene solubility to reduce the amount of solvents necessary for fullerene purification.
6	Minimizing energy	N/A
7	Using renewable feedstock	We identified plant-based alternative solvents besides petroleum-based solvents.
8	Avoiding unnecessary derivatization	N/A
9	Catalytic reagents are better than stoichiometric reagents	N/A
10	Avoid using undegradable chemicals	N/A
11	In-process monitoring to avoid generating hazardous materials	We used analytical chemistry (HPLC-UV) to monitor the impurity.
12	Safer substrates for accident prevention	We determined alternative non-hazardous solvents to reduce accidental release risk.

S3 - Data source for life-cycle assessment

Table S2. Data sources for material and energy used in inventory analysis

	Description	Ref.
1 2 4-trimethylbenzene	Co-production of mesitylene, xylenes, and benzene from naphtha cracking	(2)
1,8-Diazabicyclo (5.4.0)undec-7-ene	Synthesis of bicyclic amidines from caprolactam by using acrylonitrile	(3)
Linseed oil	Process modification from Refined sunflower oil (pressing), at processing, Agri-footprint 5.0; Linseed seed, Ecoinvent 3	(4)
Olive oil	Process modification from olive production, Ecoinvent 3 (4), based on information on olive oil production(5)	(4)(5)
Centrifuge	Required energy was estimated based on using industrial-scale equipment.	(6)
Mixer		(7)
Pump		(8)
Ultrasonic bath		(9)
Ultrasonic probe		(10)

S4 - Detailed methodology

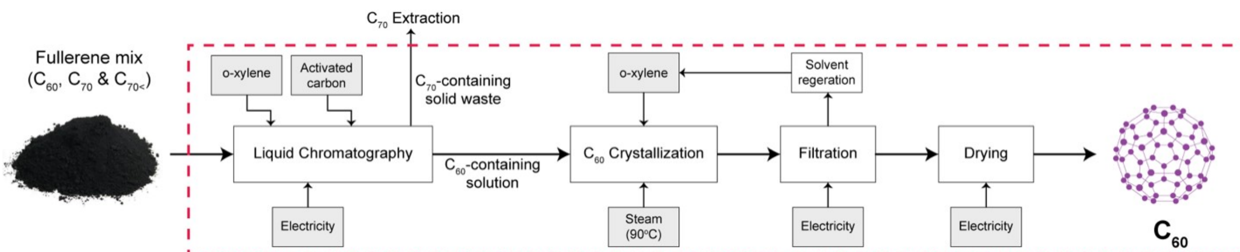

Fig. S2. The process flow of crystallization method (Kwok et al. (11)) - Red dash line shows the system boundary used for life cycle assessment (LCA). Grey boxes show input materials/energy.

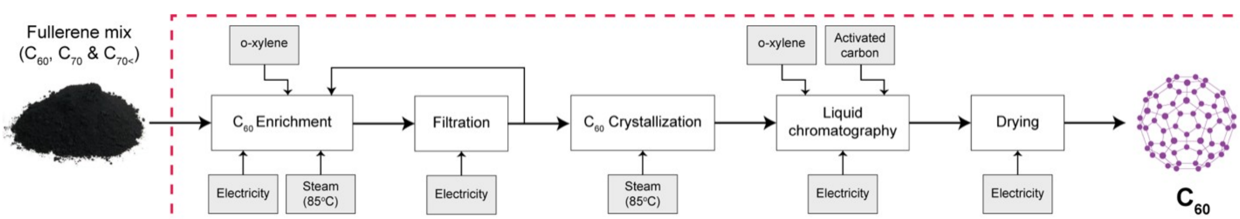

Fig. S3. The process flow of crystallization method (Grushko et al. (12)) - Red dash line shows the system boundary used for LCA. Grey boxes show input materials/energy.

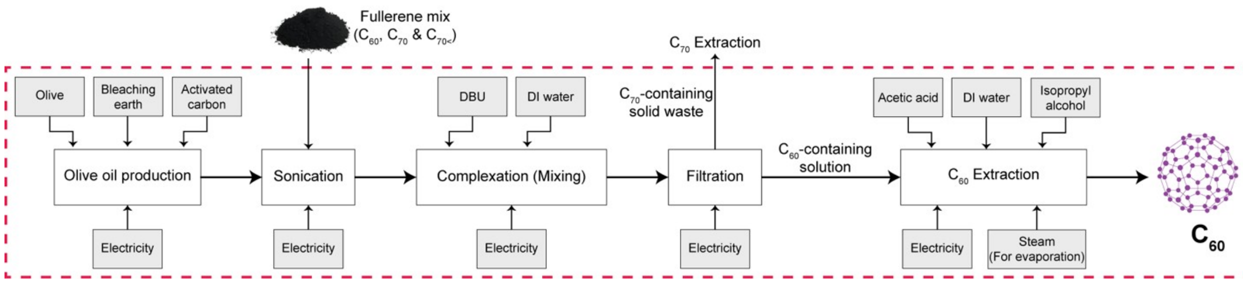

Fig. S4. Process flow for P_4 (alternative purification methods using olive oil) - Red dashed line shows the system boundary used for LCA. Grey boxes show input materials/energy. DBU: 1,8-Diazabicyclo[5.4.0]undec-7-ene.

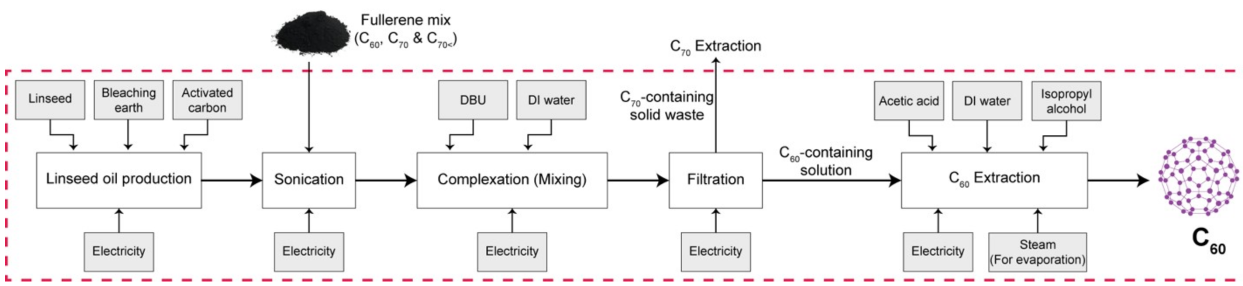

Fig. S5. Process flow for P_6 (alternative purification methods using linseed oil) - Red dashed line shows the system boundary used for LCA. Grey boxes show input materials/energy. DBU: 1,8-Diazabicyclo[5.4.0]undec-7-ene.

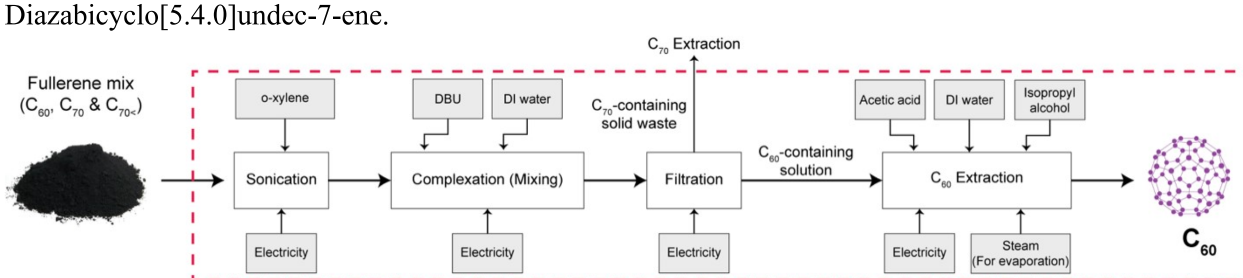

Fig. S6. Process flow for P_7 (alternative purification methods using xylene) - Red dashed line shows the system boundary used for LCA. Grey boxes show input materials/energy. DBU: 1,8-Diazabicyclo[5.4.0]undec-7-ene.

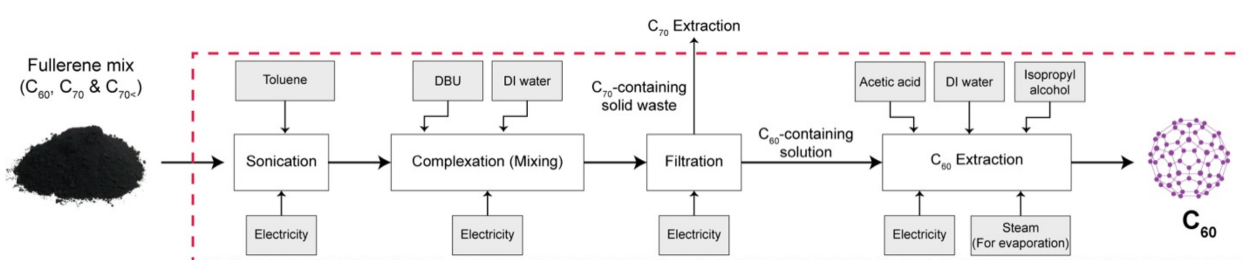

Fig. S7. Process flow for P_8 (alternative purification methods using toluene) - Red dashed line shows the system boundary used for LCA. Grey boxes show input materials/energy. DBU: 1,8-Diazabicyclo[5.4.0]undec-7-ene.

S5 – Prescreening solvents to identify replacements for TMB

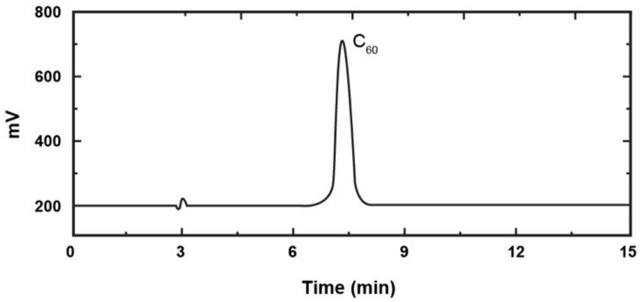

Fig. S8. HPLC analysis for the baseline process (TMB)

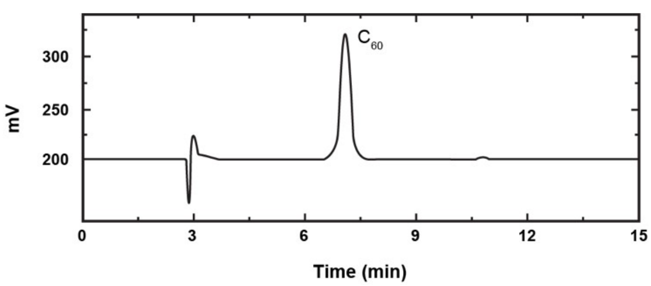

Fig. S9. HPLC analysis for alternative process P_7 (xylene)

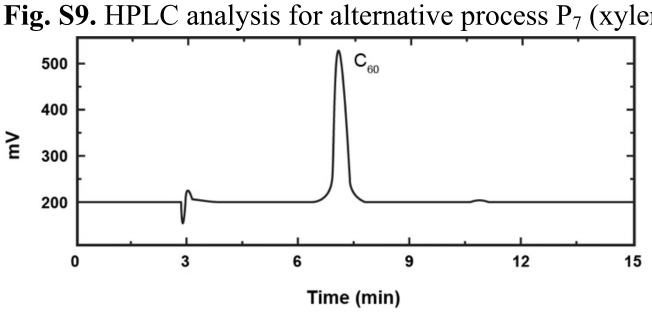

Fig. S10. HPLC analysis for alternative process P_8 (toluene)

S6 – Life cycle cost analysis

Table S3. life cycle cost analysis

Material	Unit	US$/unit	Year	Ref.
Crude Oil	kg	$0.49	2021	(13)
Bituminous Coal	kg	$0.06	2019	(14)
Lignite (brown coal)	kg	$0.02	2019	(14)
Anthracite (hard coal)	kg	$0.11	2019	(14)
Natural Gas	m3	$0.12	2020	(15)

Table S4. Production rate

Time (hr)	Rate (kg/hr)	Normalized Production Rate
5.12	0.195	1
5.27	0.190	0.972
5.45	0.183	0.939
5.25	0.190	0.975
5.45	0.183	0.939
5.25	0.190	0.975
5.27	0.190	0.972
5.27	0.190	0.972

S7 – Chemical hazard analysis

Table S5. Solvent chemical hazard scores based on NFPA.

Solvents	Health (Blue)	Flammability (Red)	Reactivity (Yellow)	Special (white)	Hazardous score	Ref.
1,2,4-trymethilbenzene (TMB)	2	2	0	0	1.33	(16)
AcOH	3	2	0	0	1.67	(16)
DBU (1,8-Diazabicyclo[5.4.0]undec-7-ene)	3	1	0	0	1.33	(17)
Heptane	1	3	0	0	1.33	(16)
IPA	2	3	0	0	1.67	(16)
Linseed oil	0	1	0	0	0.33	(18)
Olive oil	1	1	0	0	0.67	(18)
Toluene	3	3	0	0	2.00	(16)
Xylene	3	3	0	0	2.00	(16)

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