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Supplementary

1. Introduction

The supplementary material presented in this document is directly linked to the data and information presented in the article *Prospective life cycle assessment of a structural battery* by Mats Zackrisson, Christina Jönsson, Wilhelm Johannisson, Kristin Fransson, Stefan Posner, Dan Zenkert, and Göran Lindbergh. This document as such is not meant to be free standing and does not follow a traditional article structure, instead the headings are named and numbered same as its corresponding headings in the article, for which the information is applicable.

Table S1. Bill of materials for structural battery cells at initial and target levels.

Part	Constituent	Initial		Target	
		Mass [%]	Mass [g]	Mass [%]	Mass [g]
Negative electrode	Carbon fibres	8.65	674	13.97	1285
Electrolyte	SBE, see below	53.77	4194	17.65	1624
Positive electrode	Carbon fibres	8.65	674	13.97	1285
	$LiFePO_4$	10.67	832	36.82	3387
	PVDF	0.60	47	2.07	190
	Carbon black	0.72	56	2.48	228
Separator	Glass fibre	1.90	148	0.00	0
Casing	Glass fibre	10.10	788	8.75	805
	Epoxy	4.95	386	4.29	395
	Total cells incl. casing		**7800**		**9200**
Structural Battery Electrolyte, SBE	Bisphenol A dimethacrylate	56.35	2363	56.35	915
	Lithium trifluoromethanesulfonate	4.94	207	4.94	80
	Ethylene carbonate	17.28	725	17.28	281
	Dimethyl methylphosphonate	17.28	725	17.28	281
	2,2′-(Ethylenedioxy)diethanethiol	3.5	147	3.5	57
	Tris(N-nitroso-N-phenyl-hydroxylaminato) aluminum	0.05	2	0.05	1
	2,2′-Azobis(2-methylpropionitrile)	0.6	25	0.6	10

2. Materials and Methods

All materials were tracked back to the point of resource extraction, mainly by using cradle-to-gate data from the Ecoinvent 3.5 database (19). The data from Ecoinvent contains associated inputs from nature and emissions, including estimations of losses in production processes. Materials neither found in the Ecoinvent database, nor in other available databases, were modelled (from chemicals available in the databases) using molar calculations and estimations of energy use. Some materials that could not be found in the databases were replaced (in the model) with similar materials.

2.2.1. Electricity

The data sets for the electricity mixes used in the calculations are shown in **Error! Reference source not found.**.

Table S2. Electricity mixes used in the study and their climate impact.

Name of data set	Climate impact [g CO2eq/kWh]	Comment
Electricity, low voltage {ENTSO-E}| market group for | Alloc Rec, S	428	Used for propulsion of vehicle. Simulates average global use. Base case.

Name of data set	Climate impact [g CO2eq/kWh]	Comment
Electricity, low voltage {SE}| market for | Alloc Rec, S	48	Used for propulsion of vehicle. Simulates use in Sweden and future European conditions.
Electricity, high voltage {ENTSO-E}| market group for | Alloc Rec, S	414	Used for production of cell. Simulates average global production. Base case.
Electricity, high voltage {SE}| market for | Alloc Rec, S	42	Used for production of cell. Simulates production in Sweden and future European conditions.

ENTSO-E: European Network of Transmission System Operators for Electricity;
Alloc Rec, S: Allocation Recycling content, System;
SE: Sweden

2.2.2. Production of Original Traction Battery and Steel Roof

Table S3. 24 kWh NMC battery and 85 kWh NCA battery.

Characteristics	LEAF original (33Ah NMC)	Tesla original (3.1Ah NCA)
Battery capacity [kWh]	24	85
Battery mass [kg]	294	618
Batter mass w/o BMS [kg]	281	591
Energy density at cell level [Wh/kg]	155	248
Plug-to-wheel [kWh/km]	0.186	0.238
Mass of cells in pack [%]	52.2%	51.7%
Energy density at battery level [Wh/kg]	81	138
Initial design, saved battery mass [kg]	3.7	2.2
Target design, saved battery mass [kg]	12.9	7.7

The difference in energy density at cell level and at battery level is large due to that around half of the battery is not cells: it is 40% packaging, 5% battery management system (BMS), and 5% cooling system (21).

Modelling of the batteries to be replaced by the structural battery is based on a 24 kWh Lithium Nickel Manganese Cobalt oxide (NMC) battery for Nissan LEAF and on a 85 kWh Lithium Nickel Cobalt Aluminium oxide (NCA) battery used in Tesla model S. The respective BOM is given in the tables below.

The BOM-list for the original 33 Ah Nissan LEAF NMC cell was constructed by using data from (Ellingsen et al., 2013) for a smaller NMC cell (20 Ah) and scaling it to a 33 Ah cell by distributing the known total weight of the 33 Ah cell in the same proportions as the 20 Ah cell. The results are shown in the table below.

Table S4. BOM-list for 33 Ah LEAF original NMC cell (from AESC).

Part of cell	Material	Ellingsen	LEAF original
		%	Weight (g)
Cathode	NMC	35.84	286.7
Cathode	PVDF	1.41	11.3
Cathode	Carbon black	0.71	5.7
Cathode	Aluminium foil	4.91	39.3
Anode	Copper	22.25	178.0
Anode	Graphite	15.71	125.7
Anode	CMC	0.33	2.6
Anode	PAA	0.33	2.6
Separator	PP separator	2.16	17.3
Electrolyte total	$LiPF_6$ in EC: DEC:VC	15.71	125.7
Electrolyte	$LiPF_6$ (11%)		13.8

Part of cell	Material	Ellingsen	LEAF original
		%	Weight (g)
Electrolyte	Ethylene carbonate (48%)		60.3
Electrolyte	Diethyl carbonate (39%)		49.0
Electrolyte	Vinylene carbonate 2%)		2.5
Housing total		0.65	5.2
Housing	Aluminium (30%)		1.6
Housing	Polypropylene (30%)		1.6
Housing	Nickel (40%)		2.1
Total mass (g)		100	800

The BOM-lists for the original 3.1 Ah Tesla NCA cell was constructed by using data from (Bauer, 2010) for a NCA cell (20 Ah) and scaling it to a 3.1 Ah cell by distributing the known total weight of the 3.1 Ah cell in the same proportions as the 20 Ah cell. The results are shown in the table below. The 20 Ah NCA cell modelled by Bauer was a pouch cell while the Tesla cell has a cylindrical shell, assumed to be in aluminium.

Table S5. BOM-list for 3.1 Ah Tesla original NCA cell (NCR18650A from Panasonic).

Part of Cell	Material	Bauer	Tesla original
		%	Weight (g)
Cathode	NCA	27.5	11.6
Cathode	Aluminium foil	7.5	3.1
Binder	PVDF	7	3.1
Anode	Copper	14.8	6.3
Anode	Graphite	19.6	8.3
Connection	Nickel	0.3	0.1
Separator	PP separator	4.2	1.8
Electrolyte total	$LiPF_6$ in EC:DEC	18.6	7.8
Electrolyte	$LiPF_6$	11.8	
Electrolyte	Ethylene carbonate	44.1	
Electrolyte	Diethyl carbonate	44.1	
Housing	Aluminium		2.8
Total mass (g)		100	45

As an example, 0.32 kWh structural battery at initial level can replace 0.32 kWh/24 kWh NMC battery with a mass of 0.32 kWh/24 kWh*281 kg=3.75 kg. Thus, 0.32 kWh structural battery corresponds to that 3.7 kg of NMC battery does not need to be produced and the mass is avoided during use. The mass savings in respective battery are given in **Error! Reference source not found.**.

2.2.3. Production of the Structural Battery

LCA datasets for the two main constituents bisphenol A dimethacrylate and ethylene carbonate, making up 78% of the SBE, were found in the Ecoinvent database. The remaining SBE ingredients were modelled as average organic or inorganic chemicals, see **Error! Reference source not found.**.

Table S6. Life cycle model for structural battery electrolyte.

Constituent	LCA process name	Comment
Bisphenol A dimethacrylate	Bisphenol A epoxy based vinyl ester resin {GLO}| market for | Cut-off, S	56% of SBE.
Lithium trifluoro-methanesulfonate	Chemical, inorganic {GLO}| market for chemicals, inorganic | Cut-off, S	5% of SBE. This is a salt so the closest approximation is inorganic chemicals.
Ethylene carbonate	Ethylene carbonate {GLO}| market for | Cut-off, S	17% of SBE.

Constituent	LCA process name	Comment
Dimethyl methylphosphonate	Chemical, organic {GLO}∣ market for ∣ Cut-off, S	17% of SBE. This is an organic substance so the closest approximation is organic chemicals.
2,2′-(Ethylenedioxy)-diethanethiol	Chemical, organic {GLO}∣ market for ∣ Cut-off, S	3.5% of SBE. This is an organic substance so the closest approximation is organic chemicals.
Tris(N-nitroso-N-phenyl-hydroxylaminato) aluminum	Chemical, organic {GLO}∣ market for ∣ Cut-off, S	0.05% of SBE. This is mostly an organic substance so the closest approximation is organic chemicals.
2,2′-Azobis(2-methylpropionitrile)	Chemical, organic {GLO}∣ market for ∣ Cut-off, S	0.6% of SBE. This is an organic substance so the closest approximation is organic chemicals.

2.2.4. Use Phase

The following assumptions were made about transport of materials and components in connection to both lithium cell and structural battery manufacturing and use:

- Transport from mines or recycling facilities to raw material producers, these transports are normally included in the generic data used.
- 11000 km transport (1000 km lorry and 10000 km boat) from raw material producers to cell manufacturer which are expected to be close to the battery manufacturer and car assembly plant, and thus only involve a shorter truck transport (200 km). All these transports (1200 km lorry and 10000 km boat) are included in the model for Assembly.
- 6000 km transport (1000 km lorry and 5000 km boat) from car manufacturer to user. There are many car manufacturers in the world, but customers buy their cars from all over and do not select a local production. These transports, which apply also for the steel roof, are included in the model for the use phase.

2.3. Chemical Risk Assessment – in a Life Cycle Perspective

Table S7. Risk evaluation matrix including assessment criteria for evaluation of risk based on hazard and exposure, and suggested actions for the different identified risks.

Colour	Risk in each life-cycle phase	Overall risk	Criteria	Action
	Low risk	Low risk	No hazard, low exposure, small safety measures needed, no legal requirements	No concern and no action
	Moderate skin, eye and/or respiratory risks	Moderate risk	Skin, eye and respiratory hazards, ecotoxicity, moderate to high exposure, safety measures needed, no legal requirements	Precaution
	High CMR, PBT, vPvB, and/or organ risks	More than one of CMR, PBT or legal	CMR, PBT 1-2, high exposure, safety measures needed, legal requirements	Avoid

An example of input data is demonstrated in **Error! Reference source not found.** for the chemical Bisphenol A dimethacrylate. Such information has been retrieved for all chemicals in the structural battery.

Table S8. Example of data collected for the chemical risk assessment, including name, CAS-RN, hazard statement and selected physical-chemical properties.

Property	**Data**
Chemical name	Bisphenol A dimethacrylate
Amount in structural battery [%]	56.4
Hazard classified component	4-4′-isopropylidenediphenyl dimethacrylate
Concentration of classified substance [%]	100
CAS-RN of classified component	3253-39-2
Hazard statement, (EG) nr 1272/2008	H315, H319, H335
Other hazards	None
Harmonized classification	No
Aggregation state (ambient temperature)	Solid
Function in/for structural battery	Reactant, polymerizes
Legal requirements	None

The information in Tables S9 and S10 provides information regarding the information sources that have been considered for the chemical risk assessment. In table S9, the information sources and aspects that were included in the assessment are listed. During method development a larger number of aspects were included in the assessment. In an iterative manner, some aspects were identified as overlapping and thus excluded from the final assessment methodology. These aspects are listed in Table S10. Table S11-S13 provides explanations, according to CLP, to the different hazard classification codes.

Table S9. The information sources that have been used for assessing the chemical risks.

Information source	**Type of information**	**Comments**
Bill of material for structural batteries	Amount	In relation to risk assessment the amount of a specific chemical is important especially for handling and potential exposure.
Bill of material for structural batteries	Name of chemical product	Important for identification of specific chemicals
SDS information	Hazard classified component	In the chemical product, a risk is associated only with the hazardous components
SDS information	Concentration of classified substance in chemical product	In relation to risk assessment the concentration of the classified substance in a specific chemical product is important especially for handling and potential exposure.
SDS information	CAS	The identification number of chemicals. Can be used for further search in databases.
ECHA CLP database[1]	H statement, (EG) nr 1272/2008	H statements indicates the hazard associated with the specific substance. They concern both human and ecotoxicity as well as physical risks (flammable, explosive reactive etc...
ECHA CLP database[1], ChemicAll[2] or SDS	Other hazards	In some cases, chemical products may contain by-products, or the hazardous component is related to a break-down product. Also, other potential risks reported by companies in the classification database will be captured in this part.

Information source	Type of information	Comments
ECHA CLP database[1]	Harmonised classification y/n	For chemicals there exist both harmonised and non-harmonised classification in the system. The progress in the legal system is more advanced for harmonised substances. SDS may not report un-harmonised substances equally, thus qualitative assessment of all non-harmonised has been performed.
ECHA database of registered substances[3]	Aggregation state at room temperature	In relation to risk assessment the aggregation state of a specific substance is important for exposure risks during handling. Liquid state and gaseous compounds are considered higher risks for potential exposure than solids where gas phase is more related to inhalation and liquids to dermal contact.
Battery research group	Function during production or in battery	The function of a specific chemical product is important for the knowledge of state during use phase and end-of-life. Some components will react during production and become a non-hazardous product that is part of the battery structure during use and end-of-life. Other substances will not react and remain in the same aggregation state why risks may be similar in use phase and end-of-life handling as in production phase.
ECHA https://echa.europa.eu	Legal	Current and potential coming European legislation is evaluated in order to ensure compliance. Within this aspect also pro-active approach is considered for instance substitution.

[1] https://echa.europa.eu/sv/information-on-chemicals/cl-inventory-database;
[2] http://www.kemikaliegruppen.se/ChemicALL/;
[3] https://echa.europa.eu/information-on-chemicals/registered-substances

Table S10. Information sources and aspects which were originally included in the chemical risk assessment but were excluded from the final assessment.

Information source	Type of information	Comments
SDS information	P phrases	P phrases was initially part of the evaluation. However, the outcome of the assessment was not affected by P phrases. Such instructions are though very important for chemical management and handling of the chemical products in production and end-of-life.
Human Exposure, dermal	Water solubility	In order to establish potential exposure routes, specifically for dermal exposure, water solubility of the chemical products was initially identified. However, H phrases captured these aspects well, why the final assessment method did not include specification of human exposure.
Human Exposure, inhalation	Vapour pressure	In order to establish potential exposure routes, specifically for inhalation exposure, vapour pressure of the chemical products was initially identified. However, H phrases captured these aspects well, why the final assessment method did not include specification of human exposure.
Legal work environment	Work exposure limits	Work exposure limits were initially part of the evaluation. However, the outcome of the assessment was not affected by work exposure limits since they are strongly related to hazard classification. Compliance with work environment regulations is though very important for chemical management and handling of the chemical products in production and potentially also in end-of-life.

Table S11. Physical hazard codes according to CLP.

	Physical hazards
H200	Unstable explosive
H201	Explosive; mass explosion hazard
H202	Explosive; severe projection hazard
H203	Explosive; fire, blast or projection hazard
H204	Fire or projection hazard
H205	May mass explode in fire
H206	Fire, blast or projection hazard: increased risk of explosion if desensitizing agent is reduced
H207	Fire or projection hazard: increased risk of explosion if desensitizing agent is reduced
H208	Fire hazard: increased risk of explosion if desensitizing agent is reduced
H220	Extremely flammable gas
H221	Flammable gas
H222	Extremely flammable aerosol
H223	Flammable aerosol
H224	Extremely flammable liquid and vapour
H225	Highly flammable liquid and vapour
H226	Flammable liquid and vapour
H227	Combustible liquid
H228	Flammable solid
H229	Pressurized container: may burst if heated
H230	May react explosively even in the absence of air
H231	May react explosively even in the absence of air at elevated pressure and/or temperature
H232	May ignite spontaneously if exposed to air
H240	Heating may cause an explosion
H241	Heating may cause a fire or explosion
H242	Heating may cause a fire
H250	Catches fire spontaneously if exposed to air
H251	Self-heating; may catch fire
H252	Self-heating in large quantities; may catch fire
H260	In contact with water releases flammable gases which may ignite spontaneously
H261	In contact with water releases flammable gas
H270	May cause or intensify fire; oxidizer
H271	May cause fire or explosion; strong oxidizer
H272	May intensify fire; oxidizer
H280	Contains gas under pressure; may explode if heated
H281	Contains refrigerated gas; may cause cryogenic burns or injury
H290	May be corrosive to metals

Table S12. Health hazard codes according to CLP.

	Health hazards
H300	Fatal if swallowed.
H301	Toxic if swallowed
H302	Harmful if swallowed
H303	May be harmful if swallowed
H304	May be fatal if swallowed and enters airways
H305	May be harmful if swallowed and enters airways
H310	Fatal in contact with skin
H311	Toxic in contact with skin
H312	Harmful in contact with skin
H313	May be harmful in contact with skin
H314	Causes severe skin burns and eye damage
H315	Causes skin irritation
H316	Causes mild skin irritation
H317	May cause an allergic skin reaction

H318	Causes serious eye damage
H319	Causes serious eye irritation
H320	Causes eye irritation
H330	Fatal if inhaled
H331	Toxic if inhaled
H332	Harmful if inhaled
H333	May be harmful if inhaled
H334	May cause allergy or asthma symptoms or breathing difficulties if inhaled
H335	May cause respiratory irritation
H336	May cause drowsiness or dizziness
H340	May cause genetic defects
H341	Suspected of causing genetic defects
H350	May cause cancer
H351	Suspected of causing cancer
H360	May damage fertility or the unborn child
H361	Suspected of damaging fertility or the unborn child
H361d	Suspected of damaging the unborn child
H361e	May damage the unborn child
H361f	Suspected of damaging fertility
H361g	may damage fertility
H362	May cause harm to breast-fed children
H370	Causes damage to organs
H371	May cause damage to organs
H372	Causes damage to organs through prolonged or repeated exposure
H373	May cause damage to organs through prolonged or repeated exposure

Table S13. Environmental hazard codes according to CLP.

	Environmental hazards
H400	Very toxic to aquatic life
H401	Toxic to aquatic life
H402	Harmful to aquatic life
H410	Very toxic to aquatic life with long-lasting effects
H411	Toxic to aquatic life with long-lasting effects
H412	Harmful to aquatic life with long-lasting effects
H413	May cause long-lasting harmful effects to aquatic life
H420	Harms human health and environmentally by depleting ozone
H433	Harmful to terrestrial vertebrates

3.1. Life Cycle Assessment

Results in **Error! Reference source not found.** are presented as the net difference in life cycle environmental impacts when replacing a steel roof and an equivalent part of the original battery with a structural battery roof, at target level, in a small electric vehicle. European average electricity is assumed for both production and propulsion. To obtain the net difference, the environmental impact of the reference steel roof life cycle is subtracted from the structural battery roof life cycle (the latter is often negative). If the resulting measure is negative, it means avoided impact due to the structural battery roof.

From **Error! Reference source not found.** can be seen that the structural battery roof at target level in a small EV avoids, 209 kg CO_2-eq, during the life cycle. The thickness of the arrows is proportional to the impact (red arrows) or avoidance of impacts (green arrows). Most of the savings stem from the avoided production of the NMC battery (196 kg CO_2-eq). The structural battery production impacts amount to 175 kg CO_2-eq. Avoided climate impact in the use phase due to mass savings amount to 133 kg CO_2-eq; whereof 78 kg from avoiding carrying a piece of the NMC battery and 56 kg from that the structural battery roof is lighter to carry than the steel roof. Recycling the structural battery roof avoids 37 kg CO_2-eq.

The steel roof is the reference and no use phase burdens are added to it, other than transportation of roof from manufacturing site to the customer, not shown in **Error! Reference source not found.** due to cut-off at 15% of total climate impact. Production impacts, 51 kg CO_2-eq, are offset by the avoidance of impacts, 20 kg CO_2-eq, via steel recycling.

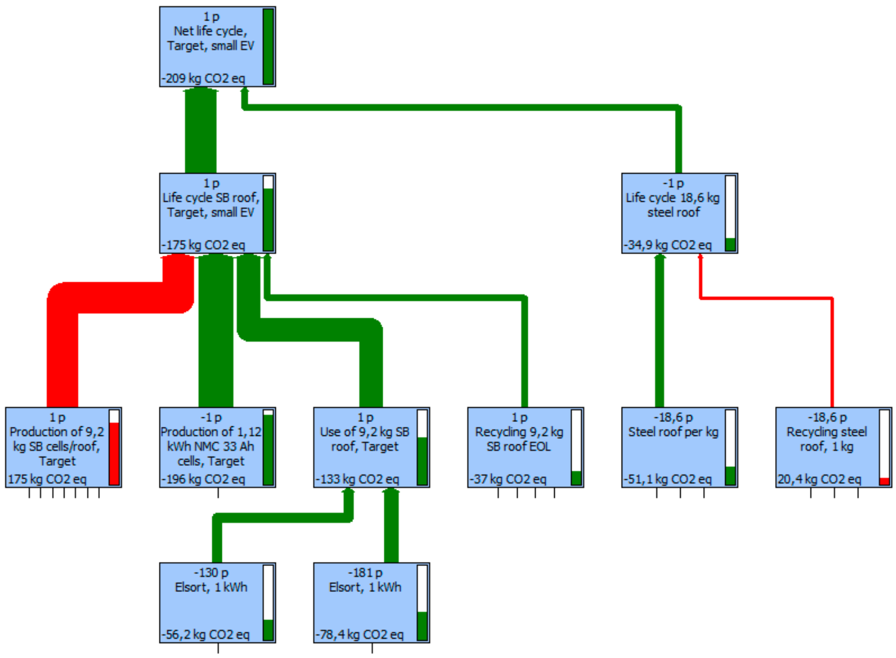

Figure S1. Net life cycle climate impacts of structural battery roof at target level in a small EV compared to steel roof, European electricity for production and propulsion. Processes contributing less than 15% not shown.

3.2. LCA Results in Perspective

With knowledge of vehicle electricity consumption, battery size, depth of discharge, weight saving and energy reduction value, the extra range for the small vehicle is calculated to 5 km or 5%: The small vehicle consumes originally 0.1863 kWh/km giving a range of 24 kWh*80%/0.1863 kWh/km = 103 km, assuming 80% depth of discharge. Since the structural battery roof is lighter than the steel roof, the 9.2 kg saved contributes with 9.2 kg*0.69 kWh/(100 kg*100 km)= =0.000635 kWh/km energy saving. The original 24 kWh battery together with the 1.1 kWh structural battery would thus give a range of (24 kWh+1.1 kWh)*80%/(0.1863 kWh/km-0.000635 kWh/km)= 108 km, i.e. the structural battery roof gives 5 km, or 5%, extra range. 5% extra range is probably worth quite a lot more than about 1% less indirect climate impact. However, gaining range means keeping the original battery intact so the climate impact avoidance would be less than 1%, for 9.2 kg substitution. But it would not be zero, since the battery roof is less heavy than the steel roof. Exchanging 10 times more steel component with structural battery would give 10 times more range, i.e. exchanging 92 kg in the small EV would give 50 km or 50% more range. For the large EV with the NCA battery the numbers are 4.5 km extra range, equivalent to 1.6% extra range for the 9.2 kg substitution.

3.3. Chemical Risk Assessment – in a Life Cycle Perspective

The chemical risk assessment includes all input chemicals to the structural battery together with relevant information regarding hazardous properties, exposure, aggregation state etc. In Figure S2, this information can be found, together with the risk assessment that consider the different life cycle phases.

Figure S2. Chemical risk assessment for chemicals in the structural battery. The table includes hazard information and assessment results for the different life cycle phases.

Chemical	Amount	Hazard classified component	Concentration*	CAS-RN classified component	H statement, (EG) nr 1272/2008	Other hazards	Harmonised classification y/n	Aggregation state at room temperature	Function during production or in battery	Legal	Production	Use	End of life	Overall	Comment
Bisphenol A dimethacrylate	56,35%	4,4'-Isopropylidene-diphenyl dimethacrylate	100%	3253-39-2	H315, H319, H335		n	Solid	Reactant, will polymerise.		Work exposure risk if dermal or eye contact or inhaled.				
Lithium trifluoromethane-sulfonate	4,94%	Synonym; Lithium triflate, Trifluoro-methanesulfonic acid	100%	33454-82-9	H302, H315, H319, H335		n	Solid, powder/salt	This will stay as a salt in liquid part of the system, this is the ion conductive salt in the battery.		Work exposure risk if dermal or eye contact or inhaled.		Work exposure risk if dermal or eye contact or inhaled.		
Ethylene carbonate	17,28%	Ethylene carbonate	100%	96-49-1	H302, H319, H373 (kidney)		n	Solid,in a solution with DMMP it's liquid.	Solvent for the ion-conductive salt.	Is currently being evaluated by ECHA.	Toxic for dermal and oral contact.	If not migration occur.	Toxic for dermal and oral contact.	Need to have good safety measures during production/end of life handling.	Substitution should be considered as a pro-active approach.
Dimethyl methylphosphonate	17,28%	Dimethyl methylphosphonate	100%	756-79-6	H319, H340, H361f (fertility)		n	Liquid	Solvent in the battery.	If reaching high volumes and harmonised classified as H340 or H361, large risk that the substance have to go through registration and authorisation process within REACH and potentially end up in Annex XVII (substances restricted under REACH),entry 29,30 due to mutagenic 1B classification H340 and reproductive toxic H361f classification.	Work exposure risk if dermal contact.	Dermal contact in liquid phase if migration occur.	Work exposure risk if dermal contact.	If reaching high volumes and harmonised classified as H340 or H361, large risk that the substance have to go through registration and authorisation process within REACH and potentially end up in Annex XVII (substances restricted under REACH),entry 29,30 due to mutagenic 1B classification H340 and reproductive toxic H361f classification.	Substitution recommended as a pro-active approach. Substitution to propylene carbonate has been initiated and is recommended from a risk perspective.
2,2′-(Ethylene-dioxy)diethanethiol	3,50%	2,2'-[1,2-Ethanediylbis(oxy)]bis(ethanethiol)	100%	14970-87-7	H302, H332, H411		n	Liquid	Polymerizing	Substances for which it is predicted (ie by the application of (Q)SARs or other evidence) that they are likely to meet the criteria for category 1 or 2 classification for carcinogenicity, mutagenicity or reproductive toxicity or the criteria in Annex XIII. **	Suspected PBT. May cause harm on the environment if released to nature.			Green since it is part of a polymer but assessed as yellow due to legal risks in the future.	Important to look for unpolymerized components. Not harmonised classified, however suspicion of persistent, toxic to the aquatic environment, toxic for reproduction. That may cause this substance to be affected by REACH legislation, particularly if becoming more high volumes.
Tris(N-hydroxy-N-nitrosophenylaminato-O,O')aluminium	0,05%	Tris(N-hydroxy-N-nitrosophenylaminato-O,O')aluminium		15305-07-4	H302, H317, H410, Potentially H350. Suspected of being Carc1B		n	Solid, powder	Part of battery, oxidising during the polymerisation. Maybe some remaining in the liquid system.		Red if harmonised classified as carcinogenic H350.		Maybe if un-oxidised residues are left at recycling safety measure have to be considered as well as handled as toxic waste.	If most is oxidised and if not classified as carcinogenic. Very low concentration in battery.	
2,2′-Azobis(2-methylpropionitrile)	0,60%	2,2'-Dimethyl-2,2'-azodipropiononitrile	100%	78-67-1	H242, H302, H332, H412		y	Solid , crystallin	Initiator creating radical groups initializing the polymerization, generally will be cross-linked to the polymer. Small parts may remain in the liquid part.	WELs NGV (Inhalable) 2 mg/m3, WELs KTV (Inhalable) 4 mg/m3.	Reactive if heated may cause a fire. Safety measures to prevent inhalation needed in production phase. Should not be released to the environment.		Maybe if residues are left at recycling safety measure have to be considered as well as handled as toxic waste.	The substance is supposed to react. Assume that nothing is left after reaction.	
Carbon fibers	32,12%	C (96%), Na and K less than 50 ppm						About 5 micron fibers, in a bundle of 6000 filament. Bundles layerd next to and on top of each other. Same lengths as the size of the car roof.	Reinforcement, active electrode and collector.		Size and shape? If fibres are generated in nano or micro scale, it may have hazaradous properties and safety measures are necessary.			Size and shape? If fibres are generated in nano or micro scale, it may have hazaradous properties and safety measures are necessary during production.	
Carbon black	0,03	C (over 96%)		215-609-9	H319, H335, H351, H373	Polycyclic aromatic hydrocarbons (PAH) are found as extractable impurities in carbon black (variable levels depending on the type of carbon black manufacture).	n	Powder	Make electrical connection between the LiFePO4-particles and carbon fibers. Mechanically bound to the coating by the PVDF.	Prop. 65. Included in CoRAP list of chemicals of concern due to expected CMR, high tonnage, fulfils exposure criteria. Work exposure limits, WELs (carbon black, dust); 3.5-10 mg/m3 DNEL workers for carbon black,Long term exp limit 2mg/m3. PNEC, Aquatice env limit 5mg/l.	PAH content Explosive, carcinogenic Safety measures important		Maybe if residues are left at recycling safety measure have to be considered as well as handled as toxic waste. Emissions of carbon black may occur during recycling/waste treatment.	Check on-going legal evaluation process. If classified as carcinogenic, this substance may be subjcet for substitution. Check PAH content.	
Acetone	300 ml	Acetone		67-64-1	H225, H319, H336		y	Liquid	Process-aid- Solvent for making the suspension of PVDF, CB and LiFePO4 particles that can be electrophoretically adhered to carbon fibers.	EC list no; 200-662-2 reg nr	Highly flammable, use proper safety measures.				
Iodine	182 mg	Iodine		7553-56-2	H312, H332, H400	According to many notifications but not included in harmonised classification H372 (Thyroid).	y	Solid, powder	Reacting with the acetone in order to create a proton, will then stay as a negative ion. The proton is naturally adhered to the other particles in the suspension giving them a positive charge.	Included as approved substance in BPR for PT 1,3,4,22. If biocidal clain, BPR must be considered.	Aquatic tox, may damage organs when repeated exposure, skin			Very small amounts. Safety measures needed when handling. Legal status should be regularly checked.	
Surfactant Triton X-100	1,2 ml	p-tertiary-Octylphenoxy polyethyl alcohol	<100%	9002-93-1	H302, H315, H318, H319, H410, H411		n	Liquid, detergent	Added to the acetone in order to make sure the particles are not clumping together in the acetone and creates a smooth suspension. Possibly by changing the surface tension. Adhere the CB and LiFePO4 to the carbon fibers.		Aquatic tox, m, skin and eye irritant.			Very small amount.	
PVDF	42,34%			24937-79-9	No notified hazards		n	Solid, powder							
LiFePO4	2,38%			15365-14-7	No notified hazards		n	Solid, powder							
Alternative: Propylene carbonate	17,28%			108-32-7	H319		y	Liquid	Solvent in the battery.		Work exposure risk if eye contact.		Work exposure risk if eye contact.		Good substitute for Dimethyl methylphosphonate since significantly lower risk.

* Concentration of classified substance in chemical

** Suspected hazardous to the aquatic environment: The Danish QSAR database contains information indicating that the substance has a 96h LC50 to fish of 55.79 mg/L; The Danish QSAR database contains information indicating that the substance has a 48h EC50 to Daphnia of 2.75 mg/L; The Danish QSAR database contains information indicating that the substance has a 96h EC50 to green algae of 1.71 mg/L # Suspected persistent in the environment: The Danish QSAR database contains information indicating that the substance is predicted as non readily biodegradable # Suspected respiratory sensitiser: The Toolbox profiler Respiratory sensitisation gives an alert for respiratory sensitisation # Suspected skin sensitiser: The Toolbox profiler Protein binding alerts for skin sensitization by OASIS v1.3 gives an alert for skin sensitisation # Suspected toxic for reproduction: CAESAR developmental toxicity model in VEGA (Q)SAR platform predicts that the chemical is Toxicant (moderate reliability).