Prospective Hazard and Toxicity Screening of Sodium-ion Battery Cathode Materials

Supplementary Information

Manuel Baumann[1], Jens Peters[2], Marcel Häringer[3], Marius Schmidt[3], Luca Schneider[3], Werner Bauer[3], Joachim R. Binder[3], Marcel Weil[1, 4]

1. Institute for Technology Assessment and Systems Analysis, KIT - ITAS, Karlsruhe (Germany);
2. University of Alcalá (UAH), Department of Economics, Alcalá de Henares, Madrid, Spain
3. Institute for Applied Materials - Energy Storage Systems, KIT – IAM-ESS, Karlsruhe (Germany)
4. Helmholtz-Institute for Electrochemical Energy Storage, KIT - HIU, Ulm (Germany)

Abstract:

Sodium-ion batteries (SiB) are considered as a serious alternative to current Lithium-ion batteries (LiBs). However, SiB are an emerging technology in an early stage of development with a wide set of potential cathode material candidates available. A major challenge is therefore to identify the most promising and sustainable cathode materials for further research and potential commercialization, considering at the same time relevant regulations such as the recent new EU Battery Regulation and Europe's chemicals strategy. Here, we provide a comprehensive hazard and toxicity screening of promising SIB cathode material that includes three different toxicity and hazard perspectives: (i) Hazard Traffic Lights (HTL), (ii) Total hazard Points (THP), and (iii) Human Toxicity Potential (HTox). Over 20 different SiB cathode compositions are screened together with three state-of-the-art LiB-cathodes for comparison reasons. Inputs such as gravimetric energy density and required precursors are based on a comprehensive literature review, own laboratory data, and calculations. All cathode active materials are analysed in a bottom-up approach. The results show clearly that the energy density is one of the most important factors determining the material demand for SiB's and correspondingly the related impacts. The screening can support a preliminary assessment of cathodes and help to substitute selected precursors if they associated with increased toxic hazards, and therefore contributes to ongoing discussions towards more sustainable batteries and their labelling.

Keywords: Sodium-Ion, Lithium-Ion, Cathode, toxicity, hazard, LCA, Carbon footprint, screening, battery

Inhalt

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1 HTP

An overview of Total Hazard Point method based on [1] is provided in Figure 1. Here only the cathode materials have been analysed based on identified precursors. Here the mass shares of each CAM are calculated in m grams of material M—. Each with a certain hazard and a corresponding lower tier of LT1, LT2, and LT3. The results are depicted in hazard points HP(g). The share of each material is set to E kWh, that can be stored in the CAM. the hazard score (HS)points are then calculated based LTs. Again, the LTs are based on hazard statements reported by more than 100 notifications from companies via the Summary of Classification and Labelling sheets from ECHA. The energy densities can be found in [2]

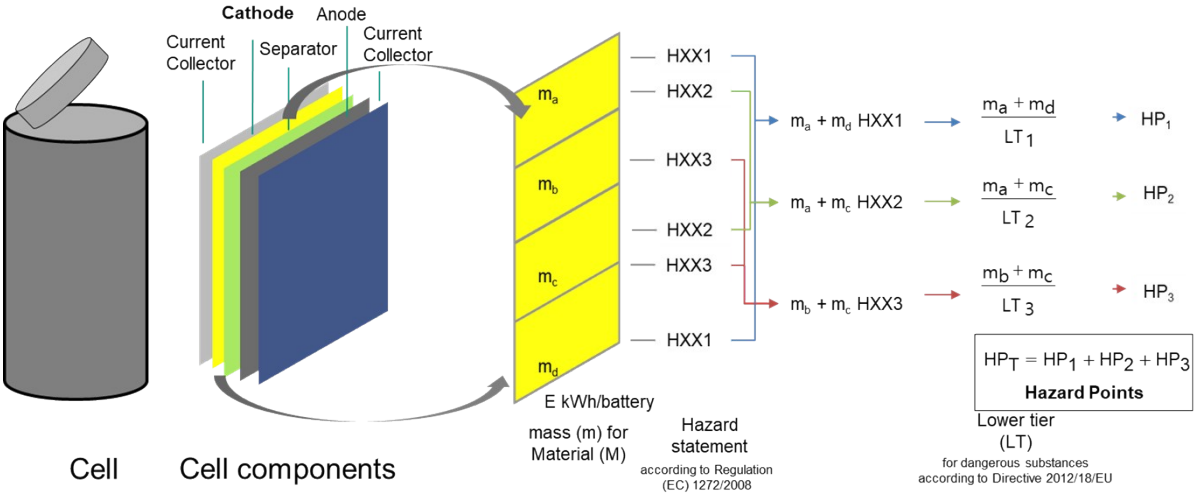


Figure 1: Overview of the THP Method adopted from [1]

2 Hazard Traffic Lights

All included substances are provided in table 1, with the corresponding CAS identifier, the used H-statements, formulas as well as links to the Summary of Classification and Labelling. In the following all THL results are provided which serve as a base for the HTP (Figure 2-32). For each of these sheets, the H-statements are identified automatically. Here all solvents are also included but are not considered in the further caclulations.

Table 1: Precursor list based on the ECHA database with corresponding H-Statement with over 100 notifications and corresponding linksl

Name EN	Name DE	CAS	H-Statement	LINK	Formula	g/mol
Sodium carbonate	Natriumcarbonat	497-19-8	H319	https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/6812	TiO2	79.866
Ammonium dihydrogenorthophosphate	Ammoniumdihydrogenphosphat	7722-76-1	H319	https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/53745	MnC2O4·2H2O	142.96
2-Propenoic acid, homopolymer	Polyacrylsäure	9003-1-4	H319, H315, H314, H340, H350	https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/45007	Ti[OCH(CH3)2]4	284.22
Ethanol		64-17-5	H225, H319, H371, H302,	https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/23129	TiO2	79.866
Oxobis(pentane-2,4-dionato-O,O')vanadium	Vanadium-Acetylacetonat	3153-26-2	H302, H315, H319, H335	https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/18634	TiO2	79.866
Orthophosphoric acid	Phsophorsäure	7664-38-2	H290, H302, H314	https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/12129	MnC2O4·2H2O	142.96
3,6,9-trioxaundecane-1,11-diol	Tetraethylenglycol	112-60-7		https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/1816	C8H18O5	194.23
Citric acid	Zitronensäurelösung	77-92-9	H319, H315,H335, H318	https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/119370	MnC2O4·2H2O	142.96
Divanadium pentaoxide	Vanadiumpentoxid	1314-62-1	H302, H332,H335,H341,H361, H411,H372	https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/103892	C8H18O5	194.23
Oxalic acid	Oxalsäure	144-62-7	H302,H312	https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/39276	C8H18O5	194.23
Dimanganese trioxide	Manganoxid	1317-34-6	H302, H312, H315, H319, H332, H335	https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/78870	C8H18O5	194.23
Natriumhydrogencarbonat	Natrium-dihygrogencarbonat	144-55-8		https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/38658	C8H18O5	194.23
Magnesium oxide	Magnesiumoxid	1309-48-4		https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/14963	MnO_2	87
Acetic acid, magnesium salt, hydrate (2:1:4)	Magnesiumacetat Tetrahydrat	605-451-2		https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/28068	TiO2	79.866
Tetrasodium	Natriumferrocyanid	13601-19-9		https://echa.europa.eu/de/information-on-	C8H18O5	194.23

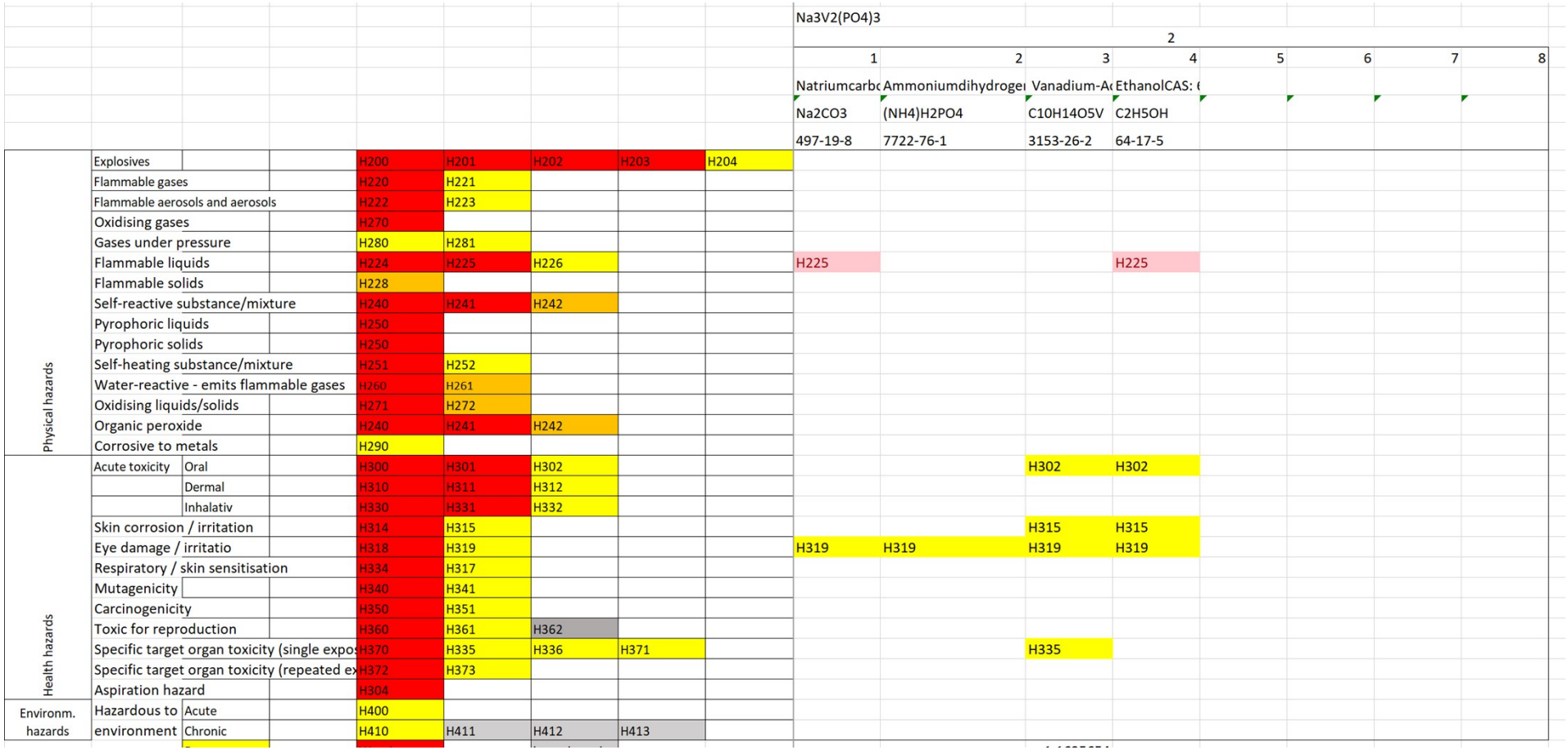
hexacyanoferrate				chemicals/cl-inventory-database/-/discli/details/66124		
hydrogen chloride	Salzsäure	7647-01-0		https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/substance/100.028.723/SELF_ALL	MnC2O4·2H2O	142.96
Sulphuric acid	Schwefelsäure	7664-93-9	H290, H314,H318,H335	https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/9111	MnC2O4·2H2O	142.96
Manganese(3+) acetate	Manganacetat	993-02-2		https://echa.europa.eu/de/substance-information/-/substanceinfo/100.012.365	Ti[OCH(CH3)2]4	284.22
Titanium dioxide	Titanoxid	13463-67-7	H351	https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/100661	C8H18O5	194.23
Potassium chloride	Kaliumchlorid	7447-40-7		https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/25989	MnC2O4·2H2O	142.96
Iron(II) oxalate	Eisen(II)-oxalat	516-03-0		https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/92500	TiO2	79.866
Argon	Argon	7440-37-1	H281, H280	https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/85110	Ar	39.948
Tetrasodium pyrophosphate	Natriumdiphosphat	7722-88-5	H319, H318,H302	https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/67932	MnC2O4·2H2O	142.96
Sodium acetate	Natriumacetat	127-09-3		https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/117757	C8H18O5	194.23
tetraethyl silicate ethyl silicate	Tetraethylorthosilicat	78-10-4	H226,H319,H332,H335	https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/124396	SiC8H20O4	208.33
Sucrose di(acetate) hexaisobutyrate	Saccharose	126-13-6		https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/85277	C8H18O5	194.23
Benzene-1,2:4,5-tetracarboxylic dianhydride	Pyromellitsäure	89-32-7	H317,H318,H334	https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/60449	NH4VO3	116.98
sodium fluoride	Natriumflourid	7681-49-4	H301,H315,H319	https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/89807	MnC2O4·2H2O	142.96
ACETIC ACID, MANGANESE(2+) SALT, TETRAHYDRATE	Mangan(II)-acetat Tetrahydrat	6156-78-1		https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/113567	TiO2	79.866
	Mangan(II)-oxalat Dihydrat	6556-16-7		N/A	TiO2	79.866
Ammonium ferrous sulfate	Ammoniumeisen(II)-sulfat	616-518-0		https://echa.europa.eu/de/information-on-	TiO2	79.866

hexahydrate				chemicals/cl-inventory-database/-/discli/details/6093		
sodium peroxide	Natriumperoxid	1313-60-6	H271, H314	https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/62772	C8H18O5	194.23
Sodium Hydroxide	Natriumhydroxid	1310-73-2	H290,H314,H318	https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/134413	C8H18O5	194.23
Diiron trioxide	Eisen(III)-oxid	1309-37-1	H319,H411	https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/18003	C8H18O5	194.23
Nickel (II)sulphate hexahydrate	Nickel(II)-sulfat	10101-97-0	H302, H315, H317, H 334, H341, H372, H400, H410, H350i, H360D	https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/9597	$NiSO_4 \cdot 6H_2O$	262.85
	Eisen(II)-sulfat	7782-63-0		https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/125344	MnC2O4·2H2O	142.96
Manganese II sulfate pentahydrate	Mangan(II)-sulfat	13465-27-5		https://echa.europa.eu/de/substance-information/-/substanceinfo/100.300.043	C8H18O5	194.23
sodium nitrite	Natriumnitrit	7632-00-0	H272,H301,H400, H301	https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/62648	MnC2O4·2H2O	142.96
Manganese dinitrate tetrahydrate	Mangan(II)-nitrat	20694-39-7		https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/207757	TiO2	79.866
Nickel(II) nitrate hexahydrate	Nickel(II)-nitrat	13478-00-7		https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/11741	C8H18O5	194.23
nickel oxide	Nickeloxid	11099-02-8	H350,H317,H372,H413,H350i	https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/131954	NiO	75
	Natriumoxalat	62-76-0		https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/14068	TiO2	79.866
	Ammoniummetavanadat	7803-55-6	H301, H315, H319, H330, H335, H341	https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/58367	MnC2O4·2H2O	142.96
	Natriumchlorid	7647-14-5	H319	https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/103945	MnC2O4·2H2O	142.96
	Mangan(II)-sulfat	10034-96-5	H373, H411	https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/55821	Ti[OCH(CH3)2]4	284.22
	Cobalt(II) sulfate heptahydrat	10026-24-1	H302, H317, H334, H341, H350, H360,H410	https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/121424	$H_{14}CoO_{11}S$	281.1
	Lithium Carbonate	554-13-2	H302, H319, H315, H318, H335, H372, H360	https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/110130	Li_2CO_3	73.89
	Ammonia, aqueous solution	1336-21-6	H301, H312,H314,H318, H335,H400	https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/128870	TiO2	79.866

Acetic acid, nickel(2+) salt, tetrahydrate	6018-89-9	H302, H317, H332,H341, H350, H360, H372	https://echa.europa.eu/information-on-chemicals/cl-inventory-database/-/discli/details/63353	C8H18O5	194.23
Lithium hydroxide	1310-66-3	H302, H314, H318	https://echa.europa.eu/substance-information/-/substanceinfo/100.013.804	TiO2	79.866
Zirconium(IV) acetylacetonate	17501-44-9		https://echa.europa.eu/substance-information/-/substanceinfo/100.037.721	C8H18O5	194.23
Diammonium dihydroxybis[lactato(2-)-O1,O2]titanate(2-)	65104-06-5	H319	https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/12318	TiO2	79.866
Titan(IV)isopropoxid	546-68-9	H226, H319, H336,	https://echa.europa.eu/de/information-on-chemicals/cl-inventory-database/-/discli/details/45270	TiO2	79.866

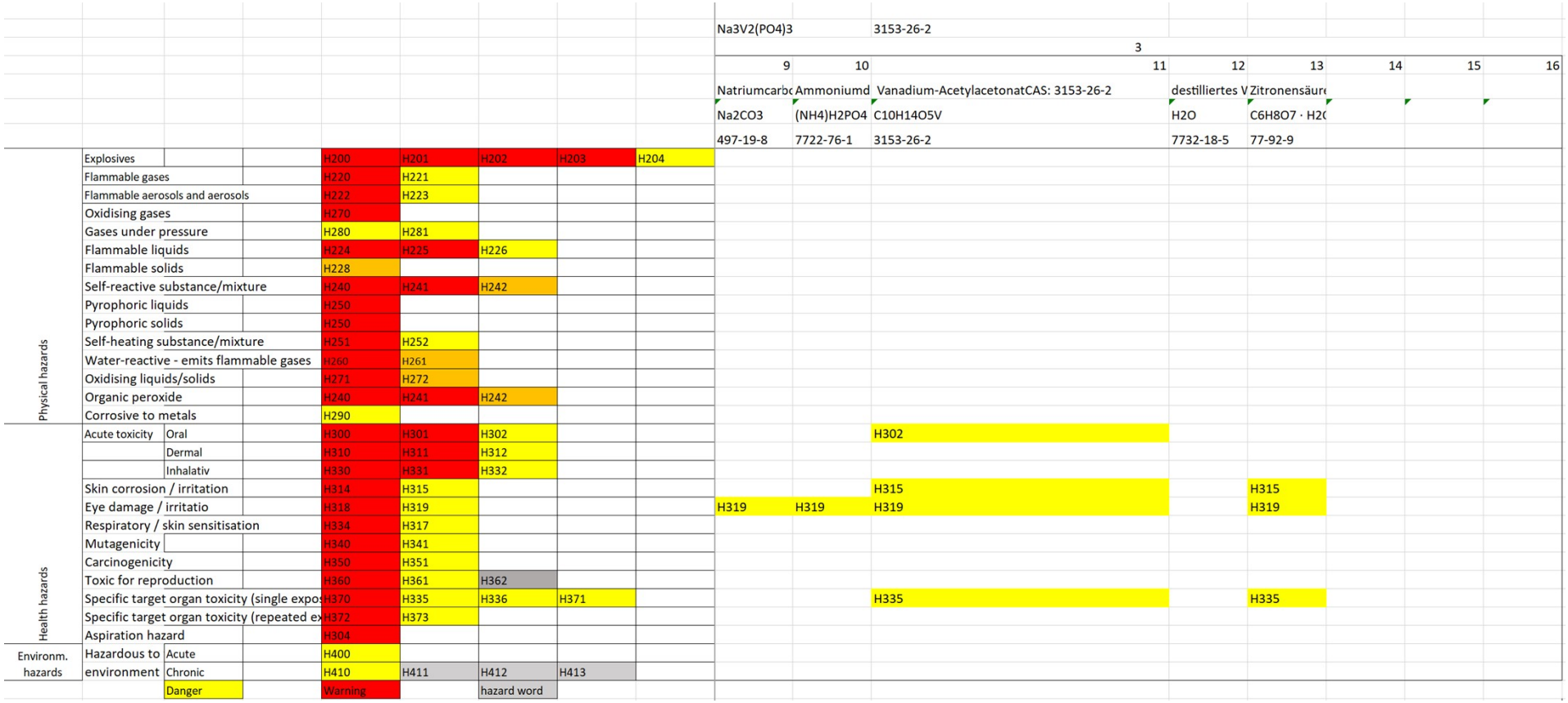
										Na3V2(PO4)3							
													1				
										1	2	3	4	5	6	7	8
										NatriumacetatCAS	Vanadium-AcetylacetonatCAS	Phosphorsäure(	Tetraethylenglycol112-60-7	Entzündbarer			
								Formula		C2H3NaO2	C10H14O5V	H3PO4	C8H18O5				
								CAS		127-09-3	3153-26-2	7664-38-2	112-60-7				
Physical hazards	Explosives			H200	H201	H202	H203	H204	H205	H206								
	Flammable gases			H220	H221												
	Flammable aerosols and aerosols			H222	H223												
	Oxidising gases			H270													
	Gases under pressure			H280	H281												
	Flammable liquids			H224	H225	H226											
	Flammable solids			H228													
	Self-reactive substance/mixture			H240	H241	H242											
	Pyrophoric liquids			H250													
	Pyrophoric solids			H250													
	Self-heating substance/mixture			H251	H252												
	Water-reactive - emits flammable gases			H260	H261												
	Oxidising liquids/solids			H271	H272												
	Organic peroxide			H240	H241	H242											
	Corrosive to metals			H290								H290					
Health hazards	Acute toxicity	Oral		H300	H301	H302						H302	H302				
		Dermal		H310	H311	H312											
		Inhalativ		H330	H331	H332											
	Skin corrosion / irritation			H314	H315							H315	H314				
	Eye damage / irritatio			H318	H319							H319					
	Respiratory / skin sensitisation			H334	H317												
	Mutagenicity			H340	H341												
	Carcinogenicity			H350	H351												
	Toxic for reproduction			H360	H361	H362											
	Specific target organ toxicity (single expos			H370	H335	H336	H371					H335					
	Specific target organ toxicity (repeated ex			H372	H373												
	Aspiration hazard			H304													
Environm. hazards	Hazardous to environment	Acute		H400													
		Chronic		H410	H411	H412	H413										
		Danger		Warning		hazard word											

Figure 2: HTL Screening for Na3V2(PO4)3 based on [3]



									Na3V2(PO4)3			
											2	
									1	2	3	4
									Natriumcarbo	Ammoniumdihydroge	Vanadium-Ac	EthanolCAS: (
									Na2CO3	(NH4)H2PO4	C10H14O5V	C2H5OH
									497-19-8	7722-76-1	3153-26-2	64-17-5
Physical hazards	Explosives			H200	H201	H202	H203	H204				
	Flammable gases			H220	H221							
	Flammable aerosols and aerosols			H222	H223							
	Oxidising gases			H270								
	Gases under pressure			H280	H281							
	Flammable liquids			H224	H225	H226			H225			H225
	Flammable solids			H228								
	Self-reactive substance/mixture			H240	H241	H242						
	Pyrophoric liquids			H250								
	Pyrophoric solids			H250								
	Self-heating substance/mixture			H251	H252							
	Water-reactive - emits flammable gases			H260	H261							
	Oxidising liquids/solids			H271	H272							
	Organic peroxide			H240	H241	H242						
	Corrosive to metals			H290								
Health hazards	Acute toxicity	Oral		H300	H301	H302					H302	H302
		Dermal		H310	H311	H312						
		Inhalativ		H330	H331	H332						
	Skin corrosion / irritation			H314	H315						H315	H315
	Eye damage / irritatio			H318	H319				H319	H319	H319	H319
	Respiratory / skin sensitisation			H334	H317							
	Mutagenicity			H340	H341							
	Carcinogenicity			H350	H351							
	Toxic for reproduction			H360	H361	H362						
	Specific target organ toxicity (single expos			H370	H335	H336	H371				H335	
	Specific target organ toxicity (repeated ex			H372	H373							
	Aspiration hazard			H304								
Environm. hazards	Hazardous to	Acute		H400								
	environment	Chronic		H410	H411	H412	H413					

Figure 3: HTL Screening for Na3V2(PO4)3 based on [4]



									Na3V2(PO4)3		3153-26-2					
											3					
									9	10	11	12	13	14	15	16
									Natriumcarbo	Ammoniumd	Vanadium-AcetylacetonatCAS: 3153-26-2	destilliertes V	Zitronensäure			
									Na2CO3	(NH4)H2PO4	C10H14O5V	H2O	C6H8O7 · H2O			
									497-19-8	7722-76-1	3153-26-2	7732-18-5	77-92-9			
Physical hazards	Explosives			H200	H201	H202	H203	H204								
	Flammable gases			H220	H221											
	Flammable aerosols and aerosols			H222	H223											
	Oxidising gases			H270												
	Gases under pressure			H280	H281											
	Flammable liquids			H224	H225	H226										
	Flammable solids			H228												
	Self-reactive substance/mixture			H240	H241	H242										
	Pyrophoric liquids			H250												
	Pyrophoric solids			H250												
	Self-heating substance/mixture			H251	H252											
	Water-reactive - emits flammable gases			H260	H261											
	Oxidising liquids/solids			H271	H272											
	Organic peroxide			H240	H241	H242										
	Corrosive to metals			H290												
Health hazards	Acute toxicity	Oral		H300	H301	H302					H302					
		Dermal		H310	H311	H312										
		Inhalativ		H330	H331	H332										
	Skin corrosion / irritation			H314	H315						H315		H315			
	Eye damage / irritatio			H318	H319				H319	H319	H319		H319			
	Respiratory / skin sensitisation			H334	H317											
	Mutagenicity			H340	H341											
	Carcinogenicity			H350	H351											
	Toxic for reproduction			H360	H361	H362										
	Specific target organ toxicity (single expo			H370	H335	H336	H371				H335		H335			
	Specific target organ toxicity (repeated ex			H372	H373											
	Aspiration hazard			H304												
Environm. hazards	Hazardous to environment	Acute		H400												
		Chronic		H410	H411	H412	H413									
		Danger		Warning		hazard word										

Figure 4: HTL Screening for Na3V2(PO4)3 based on [5]

								Na3V2(PO4)3							
								4							
								17	18	19	20	21	22	23	24
								Vanadiumpentoxid	OxalsäureCAS	destilliertes V	Natrium-dihy	GlucoseCAS:	Triethylphosp		
								V_2O_5	$C_2H_2O_4$	H_2O	$NaHCO_3$	$C_6H_{12}O_6$	$(C_2H_5O)_3PO$		
								1314-62-1	144-62-7	7732-18-5	144-55-8	50-99-7	78-40-0		
Physical hazards	Explosives			H200	H201	H202	H203	H204							
	Flammable gases			H220	H221										
	Flammable aerosols and aerosols			H222	H223										
	Oxidising gases			H270											
	Gases under pressure			H280	H281										
	Flammable liquids			H224	H225	H226									
	Flammable solids			H228											
	Self-reactive substance/mixture			H240	H241	H242									
	Pyrophoric liquids			H250											
	Pyrophoric solids			H250											
	Self-heating substance/mixture			H251	H252										
	Water-reactive - emits flammable gases			H260	H261										
	Oxidising liquids/solids			H271	H272										
	Organic peroxide			H240	H241	H242									
	Corrosive to metals			H290											
Health hazards	Acute toxicity	Oral		H300	H301	H302			H302	H302				H302	
		Dermal		H310	H311	H312				H312					
		Inhalativ		H330	H331	H332			H332						
	Skin corrosion / irritation			H314	H315										
	Eye damage / irritatio			H318	H319										
	Respiratory / skin sensitisation			H334	H317										
	Mutagenicity			H340	H341				H341						
	Carcinogenicity			H350	H351				H350						
	Toxic for reproduction			H360	H361	H362			H361						
	Specific target organ toxicity (single expos			H370	H335	H336	H371		H335						
	Specific target organ toxicity (repeated ex			H372	H373				H372						
	Aspiration hazard			H304											
Environm. hazards	Hazardous to environment	Acute		H400											
		Chronic		H410	H411	H412	H413		H411						

Figure 5: HTL Screening for Na3V2(PO4)3 based on [6]

									Na0.67[Mn0.95Mg0.05]O2						
											5				
									25	26	27	28	29	30	31	32
										ManganoxidC	Magnesiumo	Magnesiuma	destilliertes V	Natriumcarbo		
										MnO_2	MgO	Mg(CH3COO)	H2O	Na2CO3		
										1317-34-6	1309-48-4	16674-78-5	7732-18-5	497-19-8		
Physical hazards	Explosives				H200	H201	H202	H203	H204							
	Flammable gases				H220	H221										
	Flammable aerosols and aerosols				H222	H223										
	Oxidising gases				H270											
	Gases under pressure				H280	H281										
	Flammable liquids				H224	H225	H226									
	Flammable solids				H228											
	Self-reactive substance/mixture				H240	H241	H242									
	Pyrophoric liquids				H250											
	Pyrophoric solids				H250											
	Self-heating substance/mixture				H251	H252										
	Water-reactive - emits flammable gases				H260	H261										
	Oxidising liquids/solids				H271	H272										
	Organic peroxide				H240	H241	H242									
	Corrosive to metals				H290											
Health hazards	Acute toxicity	Oral			H300	H301	H302			H302						
		Dermal			H310	H311	H312			H312						
		Inhalativ			H330	H331	H332			H332						
	Skin corrosion / irritation				H314	H315				H315						
	Eye damage / irritatio				H318	H319				H319				H319		
	Respiratory / skin sensitisation				H334	H317										
	Mutagenicity				H340	H341										
	Carcinogenicity				H350	H351										
	Toxic for reproduction				H360	H361	H362									
	Specific target organ toxicity (single expo				H370	H335	H336	H371		H335						
	Specific target organ toxicity (repeated ex				H372	H373										
	Aspiration hazard				H304											
Environm. hazards	Hazardous to environment	Acute			H400											
		Chronic			H410	H411	H412	H413								
		Danger			Warning		hazard word									

Figure 6: HTL Screening for $Na_{0.67}[Mn_{0.95}Mg_{0.05}]O_2$ based on [7]

									Na2-δMn[Fe(CN)6]						
									6						
									33	34	35	36	37	38	39	40
									Natriumferro	Natriumchlor	destilliertes V	Mangan(II)-ni	EthanolCAS:			
									Na4Fe(CN)6	NaCl	H2O	$Mn(NO_3)_2$	C2H5OH			
									13601-19-9	7647-14-5	7732-18-5	10377-66-9	64-17-5			
Physical hazards	Explosives			H200	H201	H202	H203	H204								
	Flammable gases			H220	H221											
	Flammable aerosols and aerosols			H222	H223											
	Oxidising gases			H270												
	Gases under pressure			H280	H281											
	Flammable liquids			H224	H225	H226							H225			
	Flammable solids			H228												
	Self-reactive substance/mixture			H240	H241	H242										
	Pyrophoric liquids			H250												
	Pyrophoric solids			H250												
	Self-heating substance/mixture			H251	H252											
	Water-reactive - emits flammable gases			H260	H261											
	Oxidising liquids/solids			H271	H272											
	Organic peroxide			H240	H241	H242										
	Corrosive to metals			H290												
Health hazards	Acute toxicity	Oral		H300	H301	H302							H302			
		Dermal		H310	H311	H312										
		Inhalativ		H330	H331	H332										
	Skin corrosion / irritation			H314	H315											
	Eye damage / irritatio			H318	H319					H319			H319			
	Respiratory / skin sensitisation			H334	H317											
	Mutagenicity			H340	H341											
	Carcinogenicity			H350	H351											
	Toxic for reproduction			H360	H361	H362										
	Specific target organ toxicity (single expos			H370	H335	H336	H371						H371			
	Specific target organ toxicity (repeated ex			H372	H373											
	Aspiration hazard			H304												
Environm. hazards	Hazardous to environment	Acute		H400												
		Chronic		H410	H411	H412	H413									
		Danger		Warning		hazard word										

Figure 7: HTL Screening for $Na_{2-\delta}Mn[Fe(CN)_6]$ based on [8]*

									Na0.61Fe[Fe(CN)6]0.94□0.06							
												7				
									41	42	43	44	45	46	47	48
									Natriumferro							
									Na4Fe(CN)6							
									13601-19-9							
Physical hazards	Explosives			H200	H201	H202	H203	H204								
	Flammable gases			H220	H221											
	Flammable aerosols and aerosols			H222	H223											
	Oxidising gases			H270												
	Gases under pressure			H280	H281											
	Flammable liquids			H224	H225	H226										
	Flammable solids			H228												
	Self-reactive substance/mixture			H240	H241	H242										
	Pyrophoric liquids			H250												
	Pyrophoric solids			H250												
	Self-heating substance/mixture			H251	H252											
	Water-reactive - emits flammable gases			H260	H261											
	Oxidising liquids/solids			H271	H272											
	Organic peroxide			H240	H241	H242										
	Corrosive to metals			H290												
Health hazards	Acute toxicity	Oral		H300	H301	H302										
		Dermal		H310	H311	H312										
		Inhalativ		H330	H331	H332										
	Skin corrosion / irritation			H314	H315											
	Eye damage / irritatio			H318	H319											
	Respiratory / skin sensitisation			H334	H317											
	Mutagenicity			H340	H341											
	Carcinogenicity			H350	H351											
	Toxic for reproduction			H360	H361	H362										
	Specific target organ toxicity (single expos			H370	H335	H336	H371									
	Specific target organ toxicity (repeated ex			H372	H373											
	Aspiration hazard			H304												
Environm. hazards	Hazardous to environment	Acute		H400												
		Chronic		H410	H411	H412	H413									
		Danger		Warning		hazard word										

Figure 8:HTL Screening for $Na_{0.61}Fe[Fe(CN)_6]_{0.94}$[1] based on [9]

									rGO@Na0.81Fe[Fe(CN)6]0.79□0.21							
											8					
									49	50	51	52	53	54	55	56
									Natriumferrocyani	Schwefelsäur	Milli-Q-Wasse	Graphenoxid	destilliertes V			
									Na4Fe(CN)6	H2SO4			H2O			
									13601-19-9	7664-93-9			7732-18-5			
Physical hazards	Explosives				H200	H201	H202	H203	H204								
	Flammable gases				H220	H221											
	Flammable aerosols and aerosols				H222	H223											
	Oxidising gases				H270												
	Gases under pressure				H280	H281											
	Flammable liquids				H224	H225	H226										
	Flammable solids				H228												
	Self-reactive substance/mixture				H240	H241	H242										
	Pyrophoric liquids				H250												
	Pyrophoric solids				H250												
	Self-heating substance/mixture				H251	H252											
	Water-reactive - emits flammable gases				H260	H261											
	Oxidising liquids/solids				H271	H272											
	Organic peroxide				H240	H241	H242										
	Corrosive to metals				H290						H290						
Health hazards	Acute toxicity	Oral			H300	H301	H302										
		Dermal			H310	H311	H312										
		Inhalativ			H330	H331	H332										
	Skin corrosion / irritation				H314	H315					H314						
	Eye damage / irritatio				H318	H319					H318						
	Respiratory / skin sensitisation				H334	H317											
	Mutagenicity				H340	H341											
	Carcinogenicity				H350	H351											
	Toxic for reproduction				H360	H361	H362										
	Specific target organ toxicity (single expos				H370	H335	H336	H371			H335						
	Specific target organ toxicity (repeated ex				H372	H373											
	Aspiration hazard				H304												
Environm. hazards	Hazardous to environment	Acute			H400												
		Chronic			H410	H411	H412	H413									
		Danger			Warning		hazard word										

Figure 9: HTL screening for GO@$Na_{0.81}Fe[Fe(CN)_6]_{0.79}$[1] based on [10]

									Na0.9[Mn0.4Fe0.5Ti0.1]O2							
									9							
									57	58	59	60	61	62	63	64
									Natriumcarbo	Manganaceta	TitanoxidCAS	Natriumchlor	Kaliumchloric	Eisen IIIOxid		
									Na2CO3	Mn(CH3COO)	TiO2	NaCl	KCl	Fe2O3		
									497-19-8	6156-78-1	13463-67-7	7647-14-5	7447-40-7	1309-37-1		
Physical hazards	Explosives			H200	H201	H202	H203	H204								
	Flammable gases			H220	H221											
	Flammable aerosols and aerosols			H222	H223											
	Oxidising gases			H270												
	Gases under pressure			H280	H281											
	Flammable liquids			H224	H225	H226										
	Flammable solids			H228												
	Self-reactive substance/mixture			H240	H241	H242										
	Pyrophoric liquids			H250												
	Pyrophoric solids			H250												
	Self-heating substance/mixture			H251	H252											
	Water-reactive - emits flammable gases			H260	H261											
	Oxidising liquids/solids			H271	H272											
	Organic peroxide			H240	H241	H242										
	Corrosive to metals			H290												
Health hazards	Acute toxicity	Oral		H300	H301	H302										
		Dermal		H310	H311	H312										
		Inhalativ		H330	H331	H332										
	Skin corrosion / irritation			H314	H315											
	Eye damage / irritatio			H318	H319				H319			H319		H319		
	Respiratory / skin sensitisation			H334	H317											
	Mutagenicity			H340	H341											
	Carcinogenicity			H350	H351						H351					
	Toxic for reproduction			H360	H361	H362										
	Specific target organ toxicity (single expos			H370	H335	H336	H371									
	Specific target organ toxicity (repeated ex			H372	H373											
	Aspiration hazard			H304												
Environm. hazards	Hazardous to environment	Acute		H400												
		Chronic		H410	H411	H412	H413							H411		
		Danger		Warning		hazard word										

Figure 10: HTL screening for $Na_{0.9}[Mn_{0.4}Fe_{0.5}Ti_{0.1}]O_2$ based on [11]

									NaFePO4								
												10					
									65	66	67	68	69	70	71	72	
									Natriumcarbo	Eisen(II)-oxala	Ammoniumdihydrog	ArgonCAS: 74					
									Na2CO3	FeC2O4	(NH4)H2PO4	Ar					
									497-19-8	516-03-0	7722-76-1	7440-37-1					
Physical hazards	Explosives				H200	H201	H202	H203	H204									
	Flammable gases				H220	H221												
	Flammable aerosols and aerosols				H222	H223												
	Oxidising gases				H270													
	Gases under pressure				H280	H281						H281						
	Flammable liquids				H224	H225	H226											
	Flammable solids				H228													
	Self-reactive substance/mixture				H240	H241	H242											
	Pyrophoric liquids				H250													
	Pyrophoric solids				H250													
	Self-heating substance/mixture				H251	H252												
	Water-reactive - emits flammable gases				H260	H261												
	Oxidising liquids/solids				H271	H272												
	Organic peroxide				H240	H241	H242											
	Corrosive to metals				H290													
Health hazards	Acute toxicity	Oral			H300	H301	H302											
		Dermal			H310	H311	H312											
		Inhalativ			H330	H331	H332											
	Skin corrosion / irritation				H314	H315												
	Eye damage / irritatio				H318	H319				H319		H319						
	Respiratory / skin sensitisation				H334	H317												
	Mutagenicity				H340	H341												
	Carcinogenicity				H350	H351												
	Toxic for reproduction				H360	H361	H362											
	Specific target organ toxicity (single expos				H370	H335	H336	H371										
	Specific target organ toxicity (repeated ex				H372	H373												
	Aspiration hazard				H304													
Environm. hazards	Hazardous to	Acute			H400													
	environment	Chronic			H410	H411	H412	H413										
		Danger			Warning		hazard word											

Figure 11: HTL screening for $NaFePO_4$ based on [12]

									Na4MnFe2(PO4)(P2O7)							
												11				
									73	74	75	76	77	78	79	80
									NatriumdiphosphatC/	Manganoxala	Natriumdiph	AcetonCAS: 6	Pyromellitsäu	Eisen(II)-oxal		
									Na4P2O7	MnC2O4·2H2	Na4P2O7			FeC2O4		
									7722-88-5	640-67-5	7722-88-5	67-64-1	38116	516-03-0		
Physical hazards	Explosives			H200	H201	H202	H203	H204								
	Flammable gases			H220	H221											
	Flammable aerosols and aerosols			H222	H223											
	Oxidising gases			H270												
	Gases under pressure			H280	H281											
	Flammable liquids			H224	H225	H226						H225				
	Flammable solids			H228												
	Self-reactive substance/mixture			H240	H241	H242										
	Pyrophoric liquids			H250												
	Pyrophoric solids			H250												
	Self-heating substance/mixture			H251	H252											
	Water-reactive - emits flammable gases			H260	H261											
	Oxidising liquids/solids			H271	H272											
	Organic peroxide			H240	H241	H242										
	Corrosive to metals			H290												
Health hazards	Acute toxicity	Oral		H300	H301	H302			H302							
		Dermal		H310	H311	H312										
		Inhalativ		H330	H331	H332										
	Skin corrosion / irritation			H314	H315											
	Eye damage / irritatio			H318	H319				H319		H319	H319				
	Respiratory / skin sensitisation			H334	H317											
	Mutagenicity			H340	H341											
	Carcinogenicity			H350	H351											
	Toxic for reproduction			H360	H361	H362										
	Specific target organ toxicity (single expos			H370	H335	H336	H371					H336				
	Specific target organ toxicity (repeated ex			H372	H373											
	Aspiration hazard			H304												
Environm. hazards	Hazardous to	Acute		H400												
	environment	Chronic		H410	H411	H412	H413									
		Danger		Warning		hazard word										

*Figure 12: HTL screening for $Na_4MnFe_2(PO_4)(P_2O_7)$** based on [13]*

									Na2FeSiO4							
												12				
									81	82	83	84	85	86	87	88
									Eisen(II)-oxal	Natriumaceta	Zitronensäur	Tetraethylort	SaccharoseCAS: 57-50-1	ArgonCAS: 74		
									FeC2O4	C2H3NaO2	C6H8O7 · H2(	SiC8H20O4		Ar		
									516-03-0	127-09-3	77-92-9	78-10-4	57-50-1	7440-37-1		
Physical hazards	Explosives			H200	H201	H202	H203	H204								
	Flammable gases			H220	H221											
	Flammable aerosols and aerosols			H222	H223											
	Oxidising gases			H270												
	Gases under pressure			H280	H281									H281		
	Flammable liquids			H224	H225	H226						H226				
	Flammable solids			H228												
	Self-reactive substance/mixture			H240	H241	H242										
	Pyrophoric liquids			H250												
	Pyrophoric solids			H250												
	Self-heating substance/mixture			H251	H252											
	Water-reactive - emits flammable gases			H260	H261											
	Oxidising liquids/solids			H271	H272											
	Organic peroxide			H240	H241	H242										
	Corrosive to metals			H290												
Health hazards	Acute toxicity	Oral		H300	H301	H302										
		Dermal		H310	H311	H312										
		Inhalativ		H330	H331	H332						H332				
	Skin corrosion / irritation			H314	H315						H315					
	Eye damage / irritatio			H318	H319						H319	H319				
	Respiratory / skin sensitisation			H334	H317											
	Mutagenicity			H340	H341											
	Carcinogenicity			H350	H351											
	Toxic for reproduction			H360	H361	H362										
	Specific target organ toxicity (single expos			H370	H335	H336	H371				H335	H335				
	Specific target organ toxicity (repeated ex			H372	H373											
	Aspiration hazard			H304												
Environm. hazards	Hazardous to environment	Acute		H400												
		Chronic		H410	H411	H412	H413									
		Danger		Warning		hazard word										

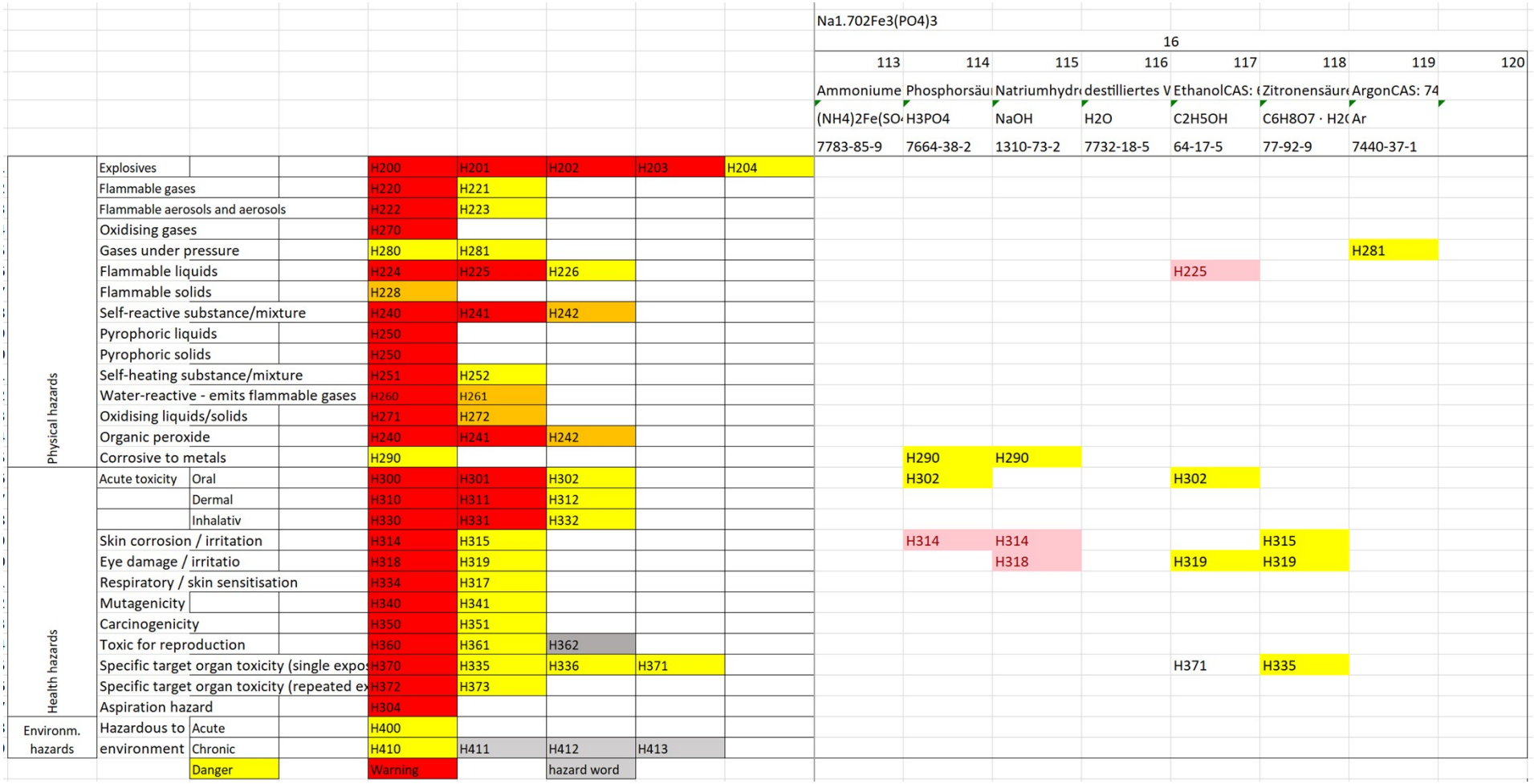
Figure 13: HTL screening for Na_2FeSiO_4 [14]*

									Na2MnSiO4							
									13							
									89	90	91	92	93	94	95	96
									Tetraethylort	EthanolCAS: (	Milli-Q-Wasse	Zitronensäur(	ManganacetatCAS: 993-0	Natriumcarbo	ArgonCAS: 74	
									SiC8H20O4	C2H5OH		C6H8O7 · H2(	Mn(CH3COO)2 · 4 H2O	Na2CO3	Ar	
									78-10-4	64-17-5		77-92-9	6156-78-1	497-19-8	7440-37-1	
Physical hazards	Explosives			H200	H201	H202	H203	H204								
	Flammable gases			H220	H221											
	Flammable aerosols and aerosols			H222	H223											
	Oxidising gases			H270												
	Gases under pressure			H280	H281										H281	
	Flammable liquids			H224	H225	H226			H226	H225						
	Flammable solids			H228												
	Self-reactive substance/mixture			H240	H241	H242										
	Pyrophoric liquids			H250												
	Pyrophoric solids			H250												
	Self-heating substance/mixture			H251	H252											
	Water-reactive - emits flammable gases			H260	H261											
	Oxidising liquids/solids			H271	H272											
	Organic peroxide			H240	H241	H242										
	Corrosive to metals			H290												
Health hazards	Acute toxicity	Oral		H300	H301	H302				H302						
		Dermal		H310	H311	H312										
		Inhalativ		H330	H331	H332			H332							
	Skin corrosion / irritation			H314	H315							H315				
	Eye damage / irritatio			H318	H319				H319	H319		H319		H319		
	Respiratory / skin sensitisation			H334	H317											
	Mutagenicity			H340	H341											
	Carcinogenicity			H350	H351											
	Toxic for reproduction			H360	H361	H362										
	Specific target organ toxicity (single expos			H370	H335	H336	H371		H335	H371		H335				
	Specific target organ toxicity (repeated ex			H372	H373											
	Aspiration hazard			H304												
Environm. hazards	Hazardous to	Acute		H400												
	environment	Chronic		H410	H411	H412	H413									
		Danger		Warning		hazard word										

Figure 14: HTL screening for Na_2MnSiO_4 based on [15]*

									Na2MnPO4F							
									14							
									97	98	99	100	101	102	103	104
									Mangan(II)-a(	Zitronensäure	destilliertes V	Natriumflour	Ammoniumd	ArgonCAS: 74		
									Mn(CH3COO)	C6H8O7 · H2(	H2O	NaF	(NH4)H2PO4	Ar		
									6156-78-1	77-92-9	7732-18-5	7681-49-4	7722-76-1	7440-37-1		
Physical hazards	Explosives			H200	H201	H202	H203	H204								
	Flammable gases			H220	H221											
	Flammable aerosols and aerosols			H222	H223											
	Oxidising gases			H270												
	Gases under pressure			H280	H281									H281		
	Flammable liquids			H224	H225	H226										
	Flammable solids			H228												
	Self-reactive substance/mixture			H240	H241	H242										
	Pyrophoric liquids			H250												
	Pyrophoric solids			H250												
	Self-heating substance/mixture			H251	H252											
	Water-reactive - emits flammable gases			H260	H261											
	Oxidising liquids/solids			H271	H272											
	Organic peroxide			H240	H241	H242										
	Corrosive to metals			H290												
Health hazards	Acute toxicity	Oral		H300	H301	H302						H301				
		Dermal		H310	H311	H312										
		Inhalativ		H330	H331	H332										
	Skin corrosion / irritation			H314	H315					H315		H315				
	Eye damage / irritatio			H318	H319					H319		H319	H319			
	Respiratory / skin sensitisation			H334	H317											
	Mutagenicity			H340	H341											
	Carcinogenicity			H350	H351											
	Toxic for reproduction			H360	H361	H362										
	Specific target organ toxicity (single expos			H370	H335	H336	H371			H335						
	Specific target organ toxicity (repeated ex			H372	H373											
	Aspiration hazard			H304												
Environm. hazards	Hazardous to environment	Acute		H400												
		Chronic		H410	H411	H412	H413									
		Danger		Warning		hazard word										

Figure 15: HTL Screening for Na_2MnPO_4F/C based on [16]*



									Na1.702Fe3(PO4)3						
									16						
									113	114	115	116	117	118	119	120
									Ammoniume	Phosphorsäu	Natriumhydr	destilliertes V	EthanolCAS: (	Zitronensäur	ArgonCAS: 74	
									(NH4)2Fe(SO	H3PO4	NaOH	H2O	C2H5OH	C6H8O7 · H2(	Ar	
									7783-85-9	7664-38-2	1310-73-2	7732-18-5	64-17-5	77-92-9	7440-37-1	
Physical hazards	Explosives			H200	H201	H202	H203	H204								
	Flammable gases			H220	H221											
	Flammable aerosols and aerosols			H222	H223											
	Oxidising gases			H270												
	Gases under pressure			H280	H281										H281	
	Flammable liquids			H224	H225	H226							H225			
	Flammable solids			H228												
	Self-reactive substance/mixture			H240	H241	H242										
	Pyrophoric liquids			H250												
	Pyrophoric solids			H250												
	Self-heating substance/mixture			H251	H252											
	Water-reactive - emits flammable gases			H260	H261											
	Oxidising liquids/solids			H271	H272											
	Organic peroxide			H240	H241	H242										
	Corrosive to metals			H290						H290	H290					
Health hazards	Acute toxicity	Oral		H300	H301	H302				H302			H302			
		Dermal		H310	H311	H312										
		Inhalativ		H330	H331	H332										
	Skin corrosion / irritation			H314	H315					H314	H314			H315		
	Eye damage / irritatio			H318	H319						H318		H319	H319		
	Respiratory / skin sensitisation			H334	H317											
	Mutagenicity			H340	H341											
	Carcinogenicity			H350	H351											
	Toxic for reproduction			H360	H361	H362										
	Specific target organ toxicity (single expos			H370	H335	H336	H371						H371	H335		
	Specific target organ toxicity (repeated ex			H372	H373											
	Aspiration hazard			H304												
Environm. hazards	Hazardous to environment	Acute		H400												
		Chronic		H410	H411	H412	H413									
		Danger		Warning		hazard word										

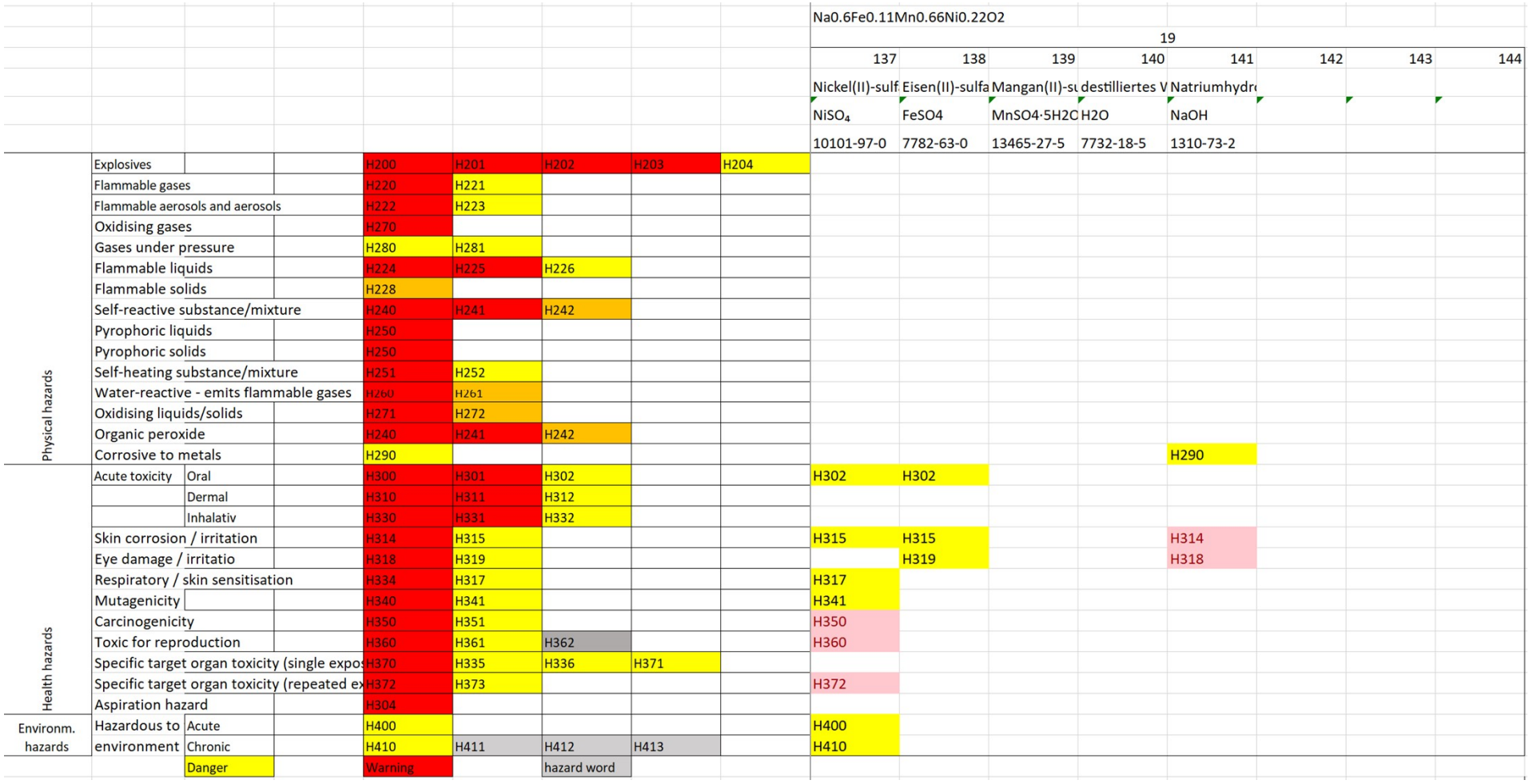
Figure 16: HTL screening for $Na_{1.702}Fe_3(PO_4)_3$ based on [17]

									NaFe0.5Mn0.5O2							
											17					
									121	122	123	124	125	126	127	128
									NatriumperoxidC	Eisen(III)-oxic	ManganoxidC					
									Na_2O_2	Fe_2O_3	MnO_2					
									1313-60-6	1309-37-1	1317-34-6					
Physical hazards	Explosives			H200	H201	H202	H203	H204								
	Flammable gases			H220	H221											
	Flammable aerosols and aerosols			H222	H223											
	Oxidising gases			H270												
	Gases under pressure			H280	H281											
	Flammable liquids			H224	H225	H226										
	Flammable solids			H228												
	Self-reactive substance/mixture			H240	H241	H242										
	Pyrophoric liquids			H250												
	Pyrophoric solids			H250												
	Self-heating substance/mixture			H251	H252											
	Water-reactive - emits flammable gases			H260	H261											
	Oxidising liquids/solids			H271	H272				H271							
	Organic peroxide			H240	H241	H242										
	Corrosive to metals			H290												
Health hazards	Acute toxicity	Oral		H300	H301	H302					H302					
		Dermal		H310	H311	H312					H312					
		Inhalativ		H330	H331	H332					H332					
	Skin corrosion / irritation			H314	H315				H314		H315					
	Eye damage / irritatio			H318	H319					H319	H319					
	Respiratory / skin sensitisation			H334	H317											
	Mutagenicity			H340	H341											
	Carcinogenicity			H350	H351											
	Toxic for reproduction			H360	H361	H362										
	Specific target organ toxicity (single expos			H370	H335	H336	H371				H335					
	Specific target organ toxicity (repeated ex			H372	H373											
	Aspiration hazard			H304												
Environm. hazards	Hazardous to	Acute		H400												
	environment	Chronic		H410	H411	H412	H413			H411						
		Danger		Warning		hazard word										

Figure 17: HTL screening for $NaFe_{0.5}Mn_{0.5}O_2$ based on [18]

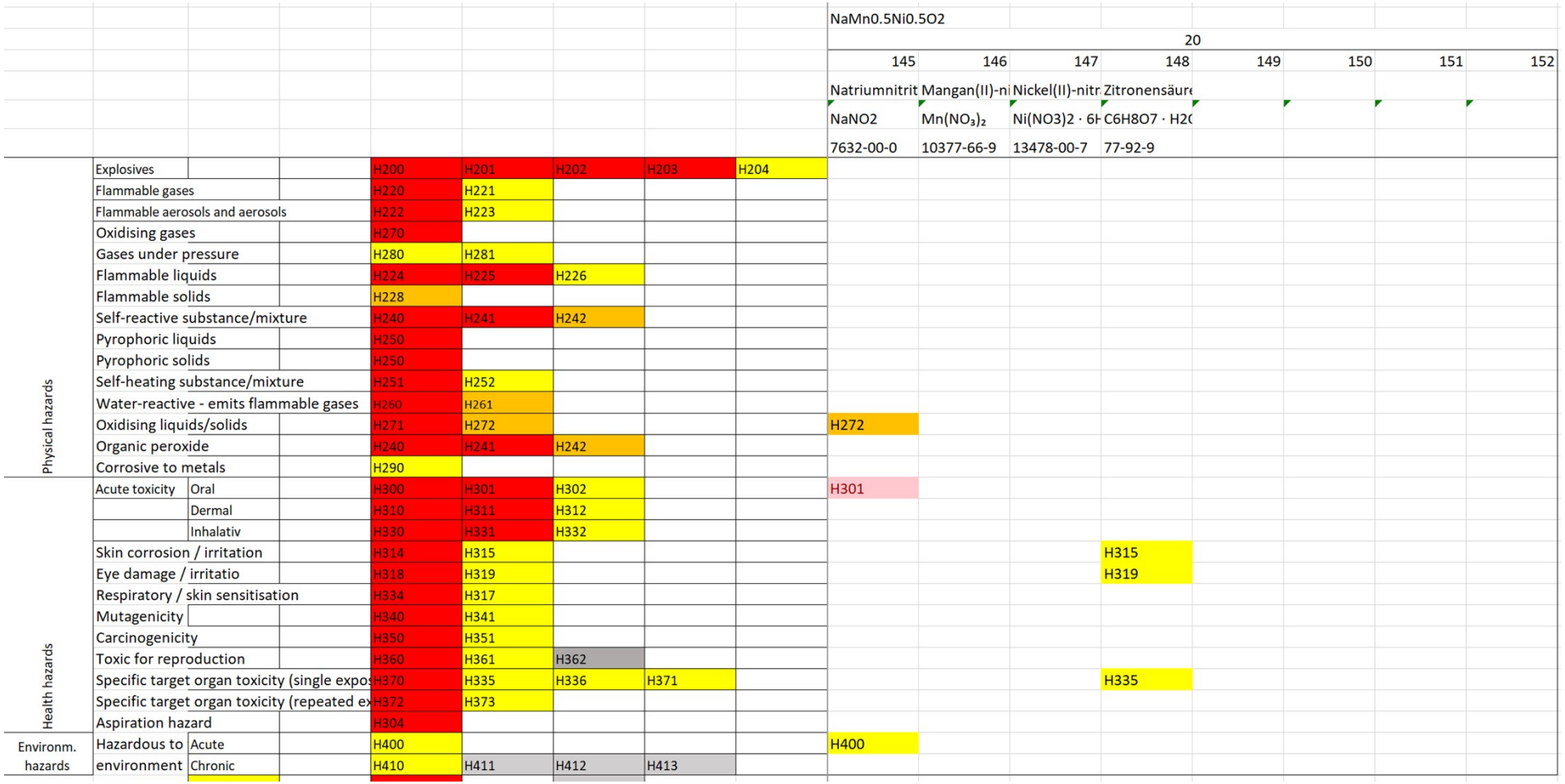
									NaMn1/3Fe1/3Ni1/3O2						
									18						
									129	130	131	132	133	134	135	136
									Nickel(II)-sulf	Eisen(II)-sulfa	Mangan(II)-su	destilliertes V	Natriumoxala	Milli-Q-Wasse	Natriumcarbo	
									$NiSO_4$	FeSO4	$MnSO_4$	H2O	Na2C2O4		Na2CO3	
									10101-97-0	7782-63-0	10034-96-5	7732-18-5	62-76-0		497-19-8	
Physical hazards	Explosives			H200	H201	H202	H203	H204								
	Flammable gases			H220	H221											
	Flammable aerosols and aerosols			H222	H223											
	Oxidising gases			H270												
	Gases under pressure			H280	H281											
	Flammable liquids			H224	H225	H226										
	Flammable solids			H228												
	Self-reactive substance/mixture			H240	H241	H242										
	Pyrophoric liquids			H250												
	Pyrophoric solids			H250												
	Self-heating substance/mixture			H251	H252											
	Water-reactive - emits flammable gases			H260	H261											
	Oxidising liquids/solids			H271	H272											
	Organic peroxide			H240	H241	H242										
	Corrosive to metals			H290												
Health hazards	Acute toxicity	Oral		H300	H301	H302			H302	H302						
		Dermal		H310	H311	H312										
		Inhalativ		H330	H331	H332										
	Skin corrosion / irritation			H314	H315				H315							
	Eye damage / irritatio			H318	H319					H319					H319	
	Respiratory / skin sensitisation			H334	H317				H317							
	Mutagenicity			H340	H341				H341							
	Carcinogenicity			H350	H351				H350							
	Toxic for reproduction			H360	H361	H362			H360							
	Specific target organ toxicity (single expos			H370	H335	H336	H371									
	Specific target organ toxicity (repeated ex			H372	H373				H372		H373					
	Aspiration hazard			H304												
Environm. hazards	Hazardous to environment	Acute		H400					H400							
		Chronic		H410	H411	H412	H413		H410		H411					
		Danger		Warning		hazard word										

Figure 18: HTL screening for $NaMn_{1/3}Fe_{1/3}Ni_{1/3}O_2$ based on [19]



									Na0.6Fe0.11Mn0.66Ni0.22O2							
											19					
									137	138	139	140	141	142	143	144
									Nickel(II)-sulf	Eisen(II)-sulfa	Mangan(II)-su	destilliertes V	Natriumhydr			
									$NiSO_4$	FeSO4	MnSO4·5H2C	H2O	NaOH			
									10101-97-0	7782-63-0	13465-27-5	7732-18-5	1310-73-2			
Physical hazards	Explosives			H200	H201	H202	H203	H204								
	Flammable gases			H220	H221											
	Flammable aerosols and aerosols			H222	H223											
	Oxidising gases			H270												
	Gases under pressure			H280	H281											
	Flammable liquids			H224	H225	H226										
	Flammable solids			H228												
	Self-reactive substance/mixture			H240	H241	H242										
	Pyrophoric liquids			H250												
	Pyrophoric solids			H250												
	Self-heating substance/mixture			H251	H252											
	Water-reactive - emits flammable gases			H260	H261											
	Oxidising liquids/solids			H271	H272											
	Organic peroxide			H240	H241	H242										
	Corrosive to metals			H290									H290			
Health hazards	Acute toxicity	Oral		H300	H301	H302			H302	H302						
		Dermal		H310	H311	H312										
		Inhalativ		H330	H331	H332										
	Skin corrosion / irritation			H314	H315				H315	H315			H314			
	Eye damage / irritatio			H318	H319					H319			H318			
	Respiratory / skin sensitisation			H334	H317				H317							
	Mutagenicity			H340	H341				H341							
	Carcinogenicity			H350	H351				H350							
	Toxic for reproduction			H360	H361	H362			H360							
	Specific target organ toxicity (single expos			H370	H335	H336	H371									
	Specific target organ toxicity (repeated ex			H372	H373				H372							
	Aspiration hazard			H304												
Environm. hazards	Hazardous to environment	Acute		H400					H400							
		Chronic		H410	H411	H412	H413		H410							
		Danger		Warning		hazard word										

Figure 19: HTL screening for $Na_{0.6}Fe_{0.11}Mn_{0.66}Ni_{0.22}O_2$ based on [20]



									NaMn0.5Ni0.5O2							
												20				
									145	146	147	148	149	150	151	152
									Natriumnitrit	Mangan(II)-ni	Nickel(II)-nitr	Zitronensäure				
									NaNO2	$Mn(NO_3)_2$	Ni(NO3)2 · 6H	C6H8O7 · H2O				
									7632-00-0	10377-66-9	13478-00-7	77-92-9				
Physical hazards	Explosives				H200	H201	H202	H203	H204								
	Flammable gases				H220	H221											
	Flammable aerosols and aerosols				H222	H223											
	Oxidising gases				H270												
	Gases under pressure				H280	H281											
	Flammable liquids				H224	H225	H226										
	Flammable solids				H228												
	Self-reactive substance/mixture				H240	H241	H242										
	Pyrophoric liquids				H250												
	Pyrophoric solids				H250												
	Self-heating substance/mixture				H251	H252											
	Water-reactive - emits flammable gases				H260	H261											
	Oxidising liquids/solids				H271	H272				H272							
	Organic peroxide				H240	H241	H242										
	Corrosive to metals				H290												
Health hazards	Acute toxicity	Oral			H300	H301	H302			H301							
		Dermal			H310	H311	H312										
		Inhalativ			H330	H331	H332										
	Skin corrosion / irritation				H314	H315						H315					
	Eye damage / irritatio				H318	H319						H319					
	Respiratory / skin sensitisation				H334	H317											
	Mutagenicity				H340	H341											
	Carcinogenicity				H350	H351											
	Toxic for reproduction				H360	H361	H362										
	Specific target organ toxicity (single expos				H370	H335	H336	H371				H335					
	Specific target organ toxicity (repeated ex				H372	H373											
	Aspiration hazard				H304												
Environm. hazards	Hazardous to environment	Acute			H400					H400							
		Chronic			H410	H411	H412	H413									

Figure 20: HTL screening for $NaMn_{0.5}Ni_{0.5}O_2$ based on [21]

									NaMnO2							
											21					
									153	154	155	156	157	158	159	160
									Natriumcarbc	ManganoxidC	ArgonCAS: 74					
									Na2CO3	MnO_2	Ar					
									497-19-8	1317-34-6	7440-37-1					
Physical hazards	Explosives			H200	H201	H202	H203	H204								
	Flammable gases			H220	H221											
	Flammable aerosols and aerosols			H222	H223											
	Oxidising gases			H270												
	Gases under pressure			H280	H281						H281					
	Flammable liquids			H224	H225	H226										
	Flammable solids			H228												
	Self-reactive substance/mixture			H240	H241	H242										
	Pyrophoric liquids			H250												
	Pyrophoric solids			H250												
	Self-heating substance/mixture			H251	H252											
	Water-reactive - emits flammable gases			H260	H261											
	Oxidising liquids/solids			H271	H272											
	Organic peroxide			H240	H241	H242										
	Corrosive to metals			H290												
Health hazards	Acute toxicity	Oral		H300	H301	H302				H302						
		Dermal		H310	H311	H312				H312						
		Inhalativ		H330	H331	H332				H332						
	Skin corrosion / irritation			H314	H315					H315						
	Eye damage / irritatio			H318	H319				H319	H319						
	Respiratory / skin sensitisation			H334	H317											
	Mutagenicity			H340	H341											
	Carcinogenicity			H350	H351											
	Toxic for reproduction			H360	H361	H362										
	Specific target organ toxicity (single expos			H370	H335	H336	H371			H335						
	Specific target organ toxicity (repeated ex			H372	H373											
	Aspiration hazard			H304												
Environm. hazards	Hazardous to environment	Acute		H400												
		Chronic		H410	H411	H412	H413									
		Danger		Warning		hazard word										

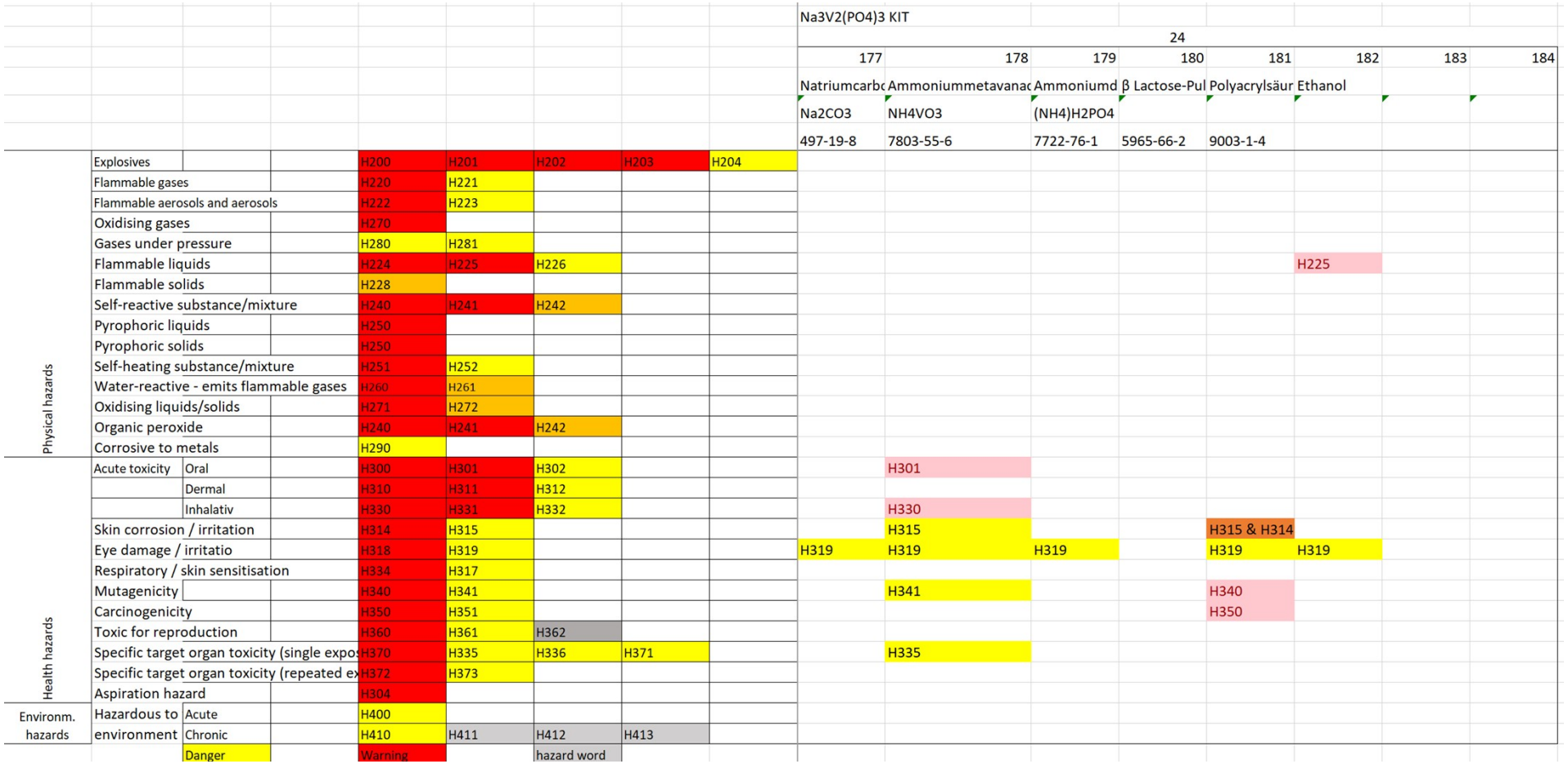
Figure 21: HTL screening for $NaMnO_2$ based on [22]

									NaMn0.3Fe0.4Ni0.3O2							
									22							
									161	162	163	164	165	166	167	168
									NaCO3Vermu	ManganoxidC	NickeloxidCA	Mangan(II)-s	Eisen(III)-oxic			
									Na2CO3	MnO_2	NiO	$MnSO_4$	Fe2O3			
									497-19-8	1317-34-6	1313-99-1	10034-96-5	1309-37-1			
Physical hazards	Explosives			H200	H201	H202	H203	H204								
	Flammable gases			H220	H221											
	Flammable aerosols and aerosols			H222	H223											
	Oxidising gases			H270												
	Gases under pressure			H280	H281											
	Flammable liquids			H224	H225	H226										
	Flammable solids			H228												
	Self-reactive substance/mixture			H240	H241	H242										
	Pyrophoric liquids			H250												
	Pyrophoric solids			H250												
	Self-heating substance/mixture			H251	H252											
	Water-reactive - emits flammable gases			H260	H261											
	Oxidising liquids/solids			H271	H272											
	Organic peroxide			H240	H241	H242										
	Corrosive to metals			H290												
Health hazards	Acute toxicity	Oral		H300	H301	H302				H302						
		Dermal		H310	H311	H312				H312						
		Inhalativ		H330	H331	H332				H332						
	Skin corrosion / irritation			H314	H315					H315						
	Eye damage / irritatio			H318	H319				H319	H319			H319			
	Respiratory / skin sensitisation			H334	H317											
	Mutagenicity			H340	H341											
	Carcinogenicity			H350	H351											
	Toxic for reproduction			H360	H361	H362										
	Specific target organ toxicity (single expos			H370	H335	H336	H371			H335						
	Specific target organ toxicity (repeated ex			H372	H373							H373				
	Aspiration hazard			H304												
Environm. hazards	Hazardous to environment	Acute		H400												
		Chronic		H410	H411	H412	H413					H411	H411			
		Danger		Warning		hazard word										

Figure 22: HTL screening for $NaMn_{0.3}Fe_{0.4}Ni_{0.3}O_2$ based on [23]

									Na0.6Fe0.20Mn0.65Ni0.15O2							
									23							
									169	170	171	172	173	174	175	176
									Natriumcarbo	ManganoxidC	NickeloxidCA	Eisen(III)-oxic				
									Na2CO3	MnO_2	NiO	Fe2O3				
									497-19-8	1317-34-6	1313-99-1	1309-37-1				
Physical hazards	Explosives				H200	H201	H202	H203	H204								
	Flammable gases				H220	H221											
	Flammable aerosols and aerosols				H222	H223											
	Oxidising gases				H270												
	Gases under pressure				H280	H281											
	Flammable liquids				H224	H225	H226										
	Flammable solids				H228												
	Self-reactive substance/mixture				H240	H241	H242										
	Pyrophoric liquids				H250												
	Pyrophoric solids				H250												
	Self-heating substance/mixture				H251	H252											
	Water-reactive - emits flammable gases				H260	H261											
	Oxidising liquids/solids				H271	H272											
	Organic peroxide				H240	H241	H242										
	Corrosive to metals				H290												
Health hazards	Acute toxicity	Oral			H300	H301	H302				H302						
		Dermal			H310	H311	H312				H312						
		Inhalativ			H330	H331	H332				H332						
	Skin corrosion / irritation				H314	H315					H315						
	Eye damage / irritatio				H318	H319				H319	H319		H319				
	Respiratory / skin sensitisation				H334	H317											
	Mutagenicity				H340	H341											
	Carcinogenicity				H350	H351											
	Toxic for reproduction				H360	H361	H362										
	Specific target organ toxicity (single expos				H370	H335	H336	H371			H335						
	Specific target organ toxicity (repeated ex				H372	H373											
	Aspiration hazard				H304												
Environm. hazards	Hazardous to environment	Acute			H400												
		Chronic			H410	H411	H412	H413				H411					
		Danger			Warning		hazard word										

Figure 23: HTL screening for $Na_{0.6}Fe_{0.20}Mn_{0.65}Ni_{0.15}O_2$ based on [24]

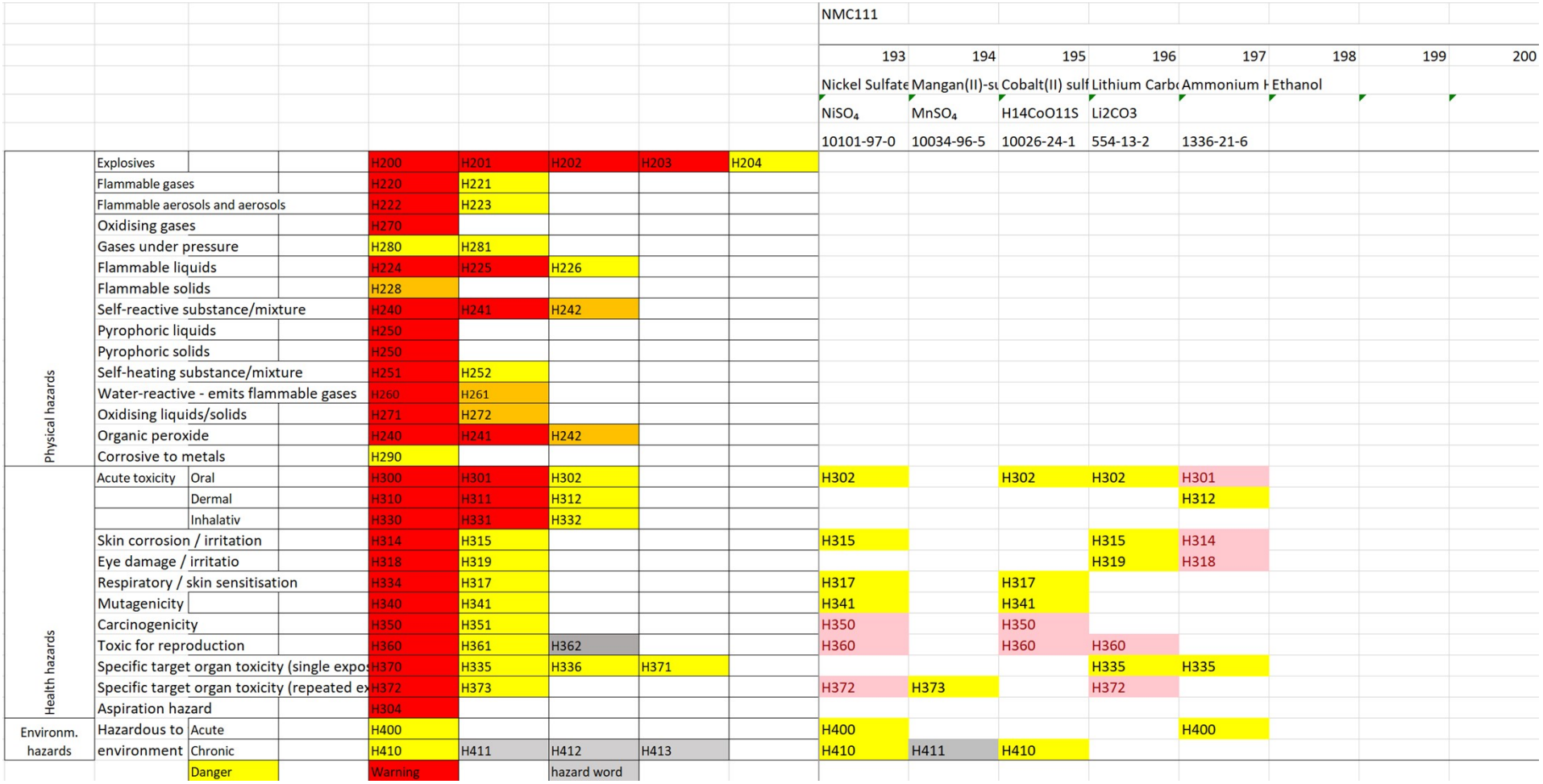


								Na3V2(PO4)3 KIT							
											24				
								177	178	179	180	181	182	183	184
								Natriumcarbo	Ammoniummetavanac	Ammoniumd	β Lactose-Pul	Polyacrylsäur	Ethanol		
								Na2CO3	NH4VO3	(NH4)H2PO4					
								497-19-8	7803-55-6	7722-76-1	5965-66-2	9003-1-4			
Physical hazards	Explosives			H200	H201	H202	H203	H204							
	Flammable gases			H220	H221										
	Flammable aerosols and aerosols			H222	H223										
	Oxidising gases			H270											
	Gases under pressure			H280	H281										
	Flammable liquids			H224	H225	H226							H225		
	Flammable solids			H228											
	Self-reactive substance/mixture			H240	H241	H242									
	Pyrophoric liquids			H250											
	Pyrophoric solids			H250											
	Self-heating substance/mixture			H251	H252										
	Water-reactive - emits flammable gases			H260	H261										
	Oxidising liquids/solids			H271	H272										
	Organic peroxide			H240	H241	H242									
	Corrosive to metals			H290											
Health hazards	Acute toxicity	Oral		H300	H301	H302				H301					
		Dermal		H310	H311	H312									
		Inhalativ		H330	H331	H332				H330					
	Skin corrosion / irritation			H314	H315					H315			H315 & H314		
	Eye damage / irritatio			H318	H319				H319	H319	H319		H319	H319	
	Respiratory / skin sensitisation			H334	H317										
	Mutagenicity			H340	H341					H341			H340		
	Carcinogenicity			H350	H351								H350		
	Toxic for reproduction			H360	H361	H362									
	Specific target organ toxicity (single expos			H370	H335	H336	H371			H335					
	Specific target organ toxicity (repeated ex			H372	H373										
	Aspiration hazard			H304											
Environm. hazards	Hazardous to	Acute		H400											
	environment	Chronic		H410	H411	H412	H413								
		Danger		Warning		hazard word									

Figure 24: HTL screening for $Na_3V_2(PO_4)_3$ based on [25]

									NMC622								
									185	186	187	188	189	190	191	192	
									Nickel Sulfate	Mangan(II)-su	Cobalt(II) sulf	Lithium Carbo	Ammonium H	Ethanol			
									$NiSO_4$	$MnSO_4$	H14CoO11S	Li2CO3					
									10101-97-0	10034-96-5	10026-24-1	554-13-2	1336-21-6				
Physical hazards	Explosives			H200	H201	H202	H203	H204									
	Flammable gases			H220	H221												
	Flammable aerosols and aerosols			H222	H223												
	Oxidising gases			H270													
	Gases under pressure			H280	H281												
	Flammable liquids			H224	H225	H226											
	Flammable solids			H228													
	Self-reactive substance/mixture			H240	H241	H242											
	Pyrophoric liquids			H250													
	Pyrophoric solids			H250													
	Self-heating substance/mixture			H251	H252												
	Water-reactive - emits flammable gases			H260	H261												
	Oxidising liquids/solids			H271	H272												
	Organic peroxide			H240	H241	H242											
	Corrosive to metals			H290													
Health hazards	Acute toxicity	Oral		H300	H301	H302			H302		H302	H302	H301				
		Dermal		H310	H311	H312							H312				
		Inhalativ		H330	H331	H332											
	Skin corrosion / irritation			H314	H315				H315			H315	H314				
	Eye damage / irritatio			H318	H319							H319	H318				
	Respiratory / skin sensitisation			H334	H317				H317		H317						
	Mutagenicity			H340	H341				H341		H341						
	Carcinogenicity			H350	H351				H350		H350						
	Toxic for reproduction			H360	H361	H362			H360		H360	H360					
	Specific target organ toxicity (single expos			H370	H335	H336	H371					H335	H335				
	Specific target organ toxicity (repeated ex			H372	H373				H372	H373		H372					
	Aspiration hazard			H304													
Environm. hazards	Hazardous to environment	Acute		H400					H400				H400				
		Chronic		H410	H411	H412	H413		H410	H411	H410						
		Danger		Warning		hazard word											

Figure 25: HTL screening for NMC 622 based on [26]



									NMC111							
									193	194	195	196	197	198	199	200
									Nickel Sulfate	Mangan(II)-su	Cobalt(II) sulf	Lithium Carb	Ammonium H	Ethanol		
									$NiSO_4$	$MnSO_4$	H14CoO11S	Li2CO3				
									10101-97-0	10034-96-5	10026-24-1	554-13-2	1336-21-6			
Physical hazards	Explosives			H200	H201	H202	H203	H204								
	Flammable gases			H220	H221											
	Flammable aerosols and aerosols			H222	H223											
	Oxidising gases			H270												
	Gases under pressure			H280	H281											
	Flammable liquids			H224	H225	H226										
	Flammable solids			H228												
	Self-reactive substance/mixture			H240	H241	H242										
	Pyrophoric liquids			H250												
	Pyrophoric solids			H250												
	Self-heating substance/mixture			H251	H252											
	Water-reactive - emits flammable gases			H260	H261											
	Oxidising liquids/solids			H271	H272											
	Organic peroxide			H240	H241	H242										
	Corrosive to metals			H290												
Health hazards	Acute toxicity	Oral		H300	H301	H302			H302		H302	H302	H301			
		Dermal		H310	H311	H312							H312			
		Inhalativ		H330	H331	H332										
	Skin corrosion / irritation			H314	H315				H315			H315	H314			
	Eye damage / irritatio			H318	H319							H319	H318			
	Respiratory / skin sensitisation			H334	H317				H317		H317					
	Mutagenicity			H340	H341				H341		H341					
	Carcinogenicity			H350	H351				H350		H350					
	Toxic for reproduction			H360	H361	H362			H360		H360	H360				
	Specific target organ toxicity (single expos			H370	H335	H336	H371					H335	H335			
	Specific target organ toxicity (repeated ex			H372	H373				H372	H373		H372				
	Aspiration hazard			H304												
Environm. hazards	Hazardous to environment	Acute		H400					H400				H400			
		Chronic		H410	H411	H412	H413		H410	H411	H410					
		Danger		Warning		hazard word										

Figure 26: HTL screening for NMC111 based on [27]

									Na0,6Ni0,22Al0,11Mn0,66O2							
									201	202	203	204	205	206	207	208
									Natriumacetat	Mangan(II)-A	Nickel(II)-Ace	Aluminium-N				
									C2H3NaO2	Mn(CH3COO)	Ni(OCOCH3)2	Al(NO3)3 · 9H				
									127-09-3	6156-78-1	6018-89-9	7784-27-2				
Physical hazards	Explosives			H200	H201	H202	H203	H204								
	Flammable gases			H220	H221											
	Flammable aerosols and aerosols			H222	H223											
	Oxidising gases			H270												
	Gases under pressure			H280	H281											
	Flammable liquids			H224	H225	H226										
	Flammable solids			H228												
	Self-reactive substance/mixture			H240	H241	H242										
	Pyrophoric liquids			H250												
	Pyrophoric solids			H250												
	Self-heating substance/mixture			H251	H252											
	Water-reactive - emits flammable gases			H260	H261											
	Oxidising liquids/solids			H271	H272											
	Organic peroxide			H240	H241	H242										
	Corrosive to metals			H290												
Health hazards	Acute toxicity	Oral		H300	H301	H302						H302				
		Dermal		H310	H311	H312										
		Inhalativ		H330	H331	H332						H332				
	Skin corrosion / irritation			H314	H315											
	Eye damage / irritatio			H318	H319											
	Respiratory / skin sensitisation			H334	H317							H317				
	Mutagenicity			H340	H341							H341				
	Carcinogenicity			H350	H351							H350				
	Toxic for reproduction			H360	H361	H362						H360				
	Specific target organ toxicity (single expos			H370	H335	H336	H371									
	Specific target organ toxicity (repeated ex			H372	H373							H372				
	Aspiration hazard			H304												
Environm. hazards	Hazardous to environment	Acute		H400												
		Chronic		H410	H411	H412	H413									
		Danger		Warning		hazard word										

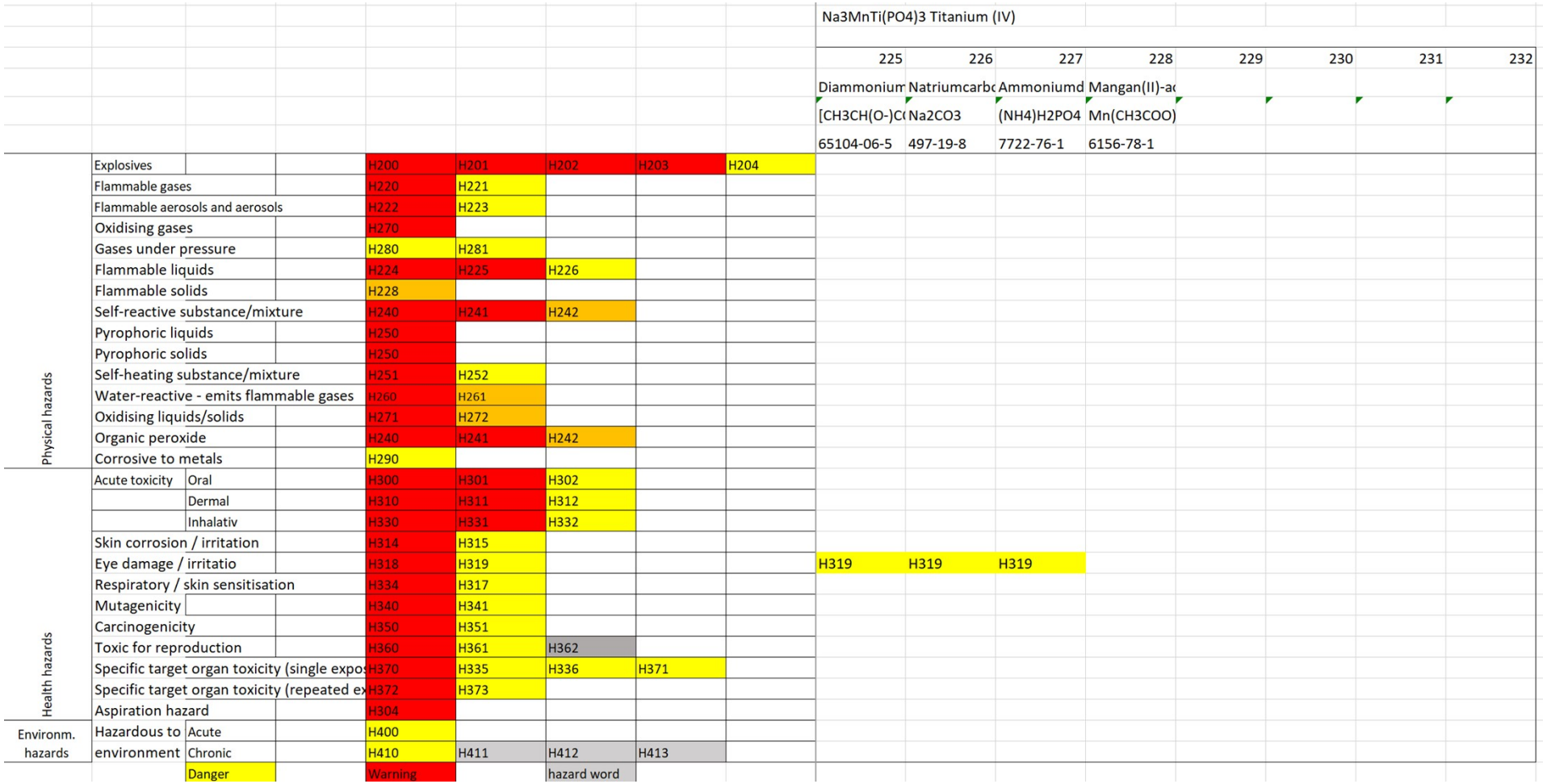
Figure 27: HTL screening for $Na_{0,6}Ni_{0,22}Al_{0,11}Mn_{0,66}O_2$ based on [28]

									LiFePO4								
									209	210	211	212	213	214	215	216	
									Lithium hydr	Phosphorsäu	Eisen(II)-sulfatCAS						
									LiOH	H3PO4	FeSO4						
									1310-66-3	7664-38-2	7782-63-0						
Physical hazards	Explosives				H200	H201	H202	H203	H204									
	Flammable gases				H220	H221												
	Flammable aerosols and aerosols				H222	H223												
	Oxidising gases				H270													
	Gases under pressure				H280	H281												
	Flammable liquids				H224	H225	H226											
	Flammable solids				H228													
	Self-reactive substance/mixture				H240	H241	H242											
	Pyrophoric liquids				H250													
	Pyrophoric solids				H250													
	Self-heating substance/mixture				H251	H252												
	Water-reactive - emits flammable gases				H260	H261												
	Oxidising liquids/solids				H271	H272												
	Organic peroxide				H240	H241	H242											
	Corrosive to metals				H290					H290								
Health hazards	Acute toxicity	Oral			H300	H301	H302			H302	H302	H302						
		Dermal			H310	H311	H312											
		Inhalativ			H330	H331	H332											
	Skin corrosion / irritation				H314	H315				H314	H314	H315						
	Eye damage / irritatio				H318	H319				H318		H319						
	Respiratory / skin sensitisation				H334	H317												
	Mutagenicity				H340	H341												
	Carcinogenicity				H350	H351												
	Toxic for reproduction				H360	H361	H362											
	Specific target organ toxicity (single expos				H370	H335	H336	H371										
	Specific target organ toxicity (repeated ex				H372	H373												
	Aspiration hazard				H304													
Environm. hazards	Hazardous to environment	Acute			H400													
		Chronic			H410	H411	H412	H413										
		Danger			Warning		hazard word											

Figure 28: HTL screening for LiFePO4, based on [29]

									Na4MnV(PO4)3							
									217	218	219	220	221	222	223	224
									Ammoniumm	Natriumcarbo	Ammoniumd	Mangan(II)-ac				
									NH4VO3	Na2CO3	(NH4)H2PO4	Mn(CH3COO)				
									7803-55-6	497-19-8	7722-76-1	6156-78-1				
Physical hazards	Explosives			H200	H201	H202	H203	H204								
	Flammable gases			H220	H221											
	Flammable aerosols and aerosols			H222	H223											
	Oxidising gases			H270												
	Gases under pressure			H280	H281											
	Flammable liquids			H224	H225	H226										
	Flammable solids			H228												
	Self-reactive substance/mixture			H240	H241	H242										
	Pyrophoric liquids			H250												
	Pyrophoric solids			H250												
	Self-heating substance/mixture			H251	H252											
	Water-reactive - emits flammable gases			H260	H261											
	Oxidising liquids/solids			H271	H272											
	Organic peroxide			H240	H241	H242										
	Corrosive to metals			H290												
Health hazards	Acute toxicity	Oral		H300	H301	H302			H301							
		Dermal		H310	H311	H312										
		Inhalativ		H330	H331	H332			H330							
	Skin corrosion / irritation			H314	H315				H315							
	Eye damage / irritatio			H318	H319				H319	H319	H319					
	Respiratory / skin sensitisation			H334	H317											
	Mutagenicity			H340	H341				H341							
	Carcinogenicity			H350	H351											
	Toxic for reproduction			H360	H361	H362										
	Specific target organ toxicity (single expos			H370	H335	H336	H371		H335							
	Specific target organ toxicity (repeated ex			H372	H373											
	Aspiration hazard			H304												
Environm. hazards	Hazardous to environment	Acute		H400												
		Chronic		H410	H411	H412	H413									
		Danger		Warning		hazard word										

Figure 29: HTL screening for $Na_4MnV(PO4)_3$-rGO based on [30]



									Na3MnTi(PO4)3 Titanium (IV)							
									225	226	227	228	229	230	231	232
									Diammonium	Natriumcarbo	Ammoniumd	Mangan(II)-ac				
									[CH3CH(O-)C(	Na2CO3	(NH4)H2PO4	Mn(CH3COO)				
									65104-06-5	497-19-8	7722-76-1	6156-78-1				
Physical hazards	Explosives				H200	H201	H202	H203	H204								
	Flammable gases				H220	H221											
	Flammable aerosols and aerosols				H222	H223											
	Oxidising gases				H270												
	Gases under pressure				H280	H281											
	Flammable liquids				H224	H225	H226										
	Flammable solids				H228												
	Self-reactive substance/mixture				H240	H241	H242										
	Pyrophoric liquids				H250												
	Pyrophoric solids				H250												
	Self-heating substance/mixture				H251	H252											
	Water-reactive - emits flammable gases				H260	H261											
	Oxidising liquids/solids				H271	H272											
	Organic peroxide				H240	H241	H242										
	Corrosive to metals				H290												
Health hazards	Acute toxicity	Oral			H300	H301	H302										
		Dermal			H310	H311	H312										
		Inhalativ			H330	H331	H332										
	Skin corrosion / irritation				H314	H315											
	Eye damage / irritatio				H318	H319				H319	H319	H319					
	Respiratory / skin sensitisation				H334	H317											
	Mutagenicity				H340	H341											
	Carcinogenicity				H350	H351											
	Toxic for reproduction				H360	H361	H362										
	Specific target organ toxicity (single expos				H370	H335	H336	H371									
	Specific target organ toxicity (repeated ex				H372	H373											
	Aspiration hazard				H304												
Environm. hazards	Hazardous to environment	Acute			H400												
		Chronic			H410	H411	H412	H413									
		Danger			Warning		hazard word										

Figure 30: HTL screening fro $Na_3MnTi(PO_4)_3$ based on [31]

									Na3MnTi(PO4)3	Titanisopropoxid							
									233	234	235	236	237	238	239	240	
									Titanisopropc	Natriumcarbc	Ammoniumd	Mangan(II)-ac					
									Ti[OCH(CH3)2	Na2CO3	(NH4)H2PO4	Mn(CH3COO)					
									546-68-9	497-19-8	7722-76-1	6156-78-1					
Physical hazards	Explosives			H200	H201	H202	H203	H204									
	Flammable gases			H220	H221												
	Flammable aerosols and aerosols			H222	H223												
	Oxidising gases			H270													
	Gases under pressure			H280	H281												
	Flammable liquids			H224	H225	H226			H226								
	Flammable solids			H228													
	Self-reactive substance/mixture			H240	H241	H242											
	Pyrophoric liquids			H250													
	Pyrophoric solids			H250													
	Self-heating substance/mixture			H251	H252												
	Water-reactive - emits flammable gases			H260	H261												
	Oxidising liquids/solids			H271	H272												
	Organic peroxide			H240	H241	H242											
	Corrosive to metals			H290													
Health hazards	Acute toxicity	Oral		H300	H301	H302											
		Dermal		H310	H311	H312											
		Inhalativ		H330	H331	H332											
	Skin corrosion / irritation			H314	H315												
	Eye damage / irritatio			H318	H319				H319	H319	H319						
	Respiratory / skin sensitisation			H334	H317												
	Mutagenicity			H340	H341												
	Carcinogenicity			H350	H351												
	Toxic for reproduction			H360	H361	H362											
	Specific target organ toxicity (single expos			H370	H335	H336	H371		H336								
	Specific target organ toxicity (repeated ex			H372	H373												
	Aspiration hazard			H304													
Environm. hazards	Hazardous to	Acute		H400													
	environment	Chronic		H410	H411	H412	H413										
		Danger		Warning		hazard word											

Figure 31: HTL screening for fro $Na_3MnTi(PO_4)_3$ based on own data.

									Na3MnZr(PO4)3							
									241	242	243	244	245	246	247	248
									Zirconium(IV)	Natriumcarbo	Ammoniumd	Mangan(II)-a				
									$C_{20}H_{28}O_8Zr$	Na2CO3	$(NH_4)H_2PO_4$	Mn(CH3COO)				
									17501-44-9	497-19-8	7722-76-1	6156-78-1				
Physical hazards	Explosives			H200	H201	H202	H203	H204								
	Flammable gases			H220	H221											
	Flammable aerosols and aerosols			H222	H223											
	Oxidising gases			H270												
	Gases under pressure			H280	H281											
	Flammable liquids			H224	H225	H226										
	Flammable solids			H228												
	Self-reactive substance/mixture			H240	H241	H242										
	Pyrophoric liquids			H250												
	Pyrophoric solids			H250												
	Self-heating substance/mixture			H251	H252											
	Water-reactive - emits flammable gases			H260	H261											
	Oxidising liquids/solids			H271	H272											
	Organic peroxide			H240	H241	H242										
	Corrosive to metals			H290												
Health hazards	Acute toxicity	Oral		H300	H301	H302										
		Dermal		H310	H311	H312										
		Inhalativ		H330	H331	H332										
	Skin corrosion / irritation			H314	H315											
	Eye damage / irritatio			H318	H319					H319	H319					
	Respiratory / skin sensitisation			H334	H317											
	Mutagenicity			H340	H341											
	Carcinogenicity			H350	H351											
	Toxic for reproduction			H360	H361	H362										
	Specific target organ toxicity (single expos			H370	H335	H336	H371									
	Specific target organ toxicity (repeated ex			H372	H373											
	Aspiration hazard			H304												
Environm. hazards	Hazardous to environment	Acute		H400												
		Chronic		H410	H411	H412	H413									
		Danger		Warning		hazard word										

Figure 32: HTL screening for $Na_3MnZr(PO_4)_3$ based on [32]

3 Total Hazard points

An screenshot of the THP calculus is provided in Figure 33. Here, the HTL evaluation is used and combined with the lower Treshholds for each substance and H-statement and calculated for each considered substance. All numeric results for the total hazard points are provided in table 2. Here all elements are considered with their corresponding impacts per kg. The results for the THP per kWh are provided in table 3.

H-Sätze	Treshholds	Gravin	Wh/kg	373		373.3		373.3		373.3	
H200	10										
H220	10										
H222	150										
H270	50										
H201	10										
H202	10										
H203	10										
H205	10										
H224	10										
H225	5000					0.349		7E-05			
H240	10										
H250	50										
H251	10										
H260	100										
H271	50										
H241	10										
H300	5										
H310	5										
H330	5										
H314	10			0.21		0.021					
H318	10										
H334	50										
H340	5										
H350	5										
H360	5										
H370	50										
H372	100									0.399	
H304	50										
H301	50										
H311	50										
H331	50										
H204	50										
H221	10										
H223	150										
H280	5000										
H281	5000										
H226	5000										
H252	50										
H290	5000			0.21		4E-05					
H302	100			1.164	0.21	0.014	1.164	0.012	1.164	0.012	0.399 1.199
H312	100										
H332	100									0.399	
H315	50			1.164		0.023	1.164	0.023	1.164	0.023	
H319	50			1.164		0.023	0.349 0.247 1.164	0.035	0.349 0.247 1.164	0.035	
H317	100										
H341	10									0.399	
H351	10										
H361	10									0.399	
H335	100			1.164		0.012	1.164	0.012	1.164	0.012	0.399
H371	100										
H373	200										
H336	100										
H400	100										
H410	100										
H228	50										
H242	50										
H261	100										
H272	50										
H242	50										
H206	10										
H362	5										
H411	200									0.399	
H412	200										
H413	200										
Total				Na3V2(PO4)3		Na3V2(PO4)3		Na3V2(PO4)3		Na3V2(PO4)3	
Per kg				69.81 23.18		**93**	7.046 4.939 69.81	**81.8**	6.976 4.939 69.81	**81.73**	97.77 11.99
Per Ah/kg						**0.791**		**0.696**		**0.695**	
Per Ah/kg						**0.847**		**0.745**		**0.744**	
Per kWh						**249.1**		**219.1**		**218.9**	
Results for THP				Na V P O			Na V P O		Na V P O		Na V P O
Per kg				69.81 23.18		93	7.046 69.81 4.939	81.8	6.976 69.81 4.939	81.73	97.77 11.99
Per kg				81.23 4.877		86.11	2.458 17.24 5.747	25.44	2.434 17.24 5.747	25.42	
Per kWh							18.87	18.87	18.69	18.69	

Figure 33: Screenshot of the THP calculation using the H-Statements and corresponding tresholds based on the HTL sheets.

Table 2: Numeric results for THP/kg

	Al	C	Co	F	Fe	Li	Mg	Mn	Na	Ni	P	Pb	Si	Ti	V	Zr
NMC111			532.1			142.6		5.197		314.2						
NMC622			216.8			141		3.116		565.2						
NaMnO2								63.27	9.642							
Na0.67[Mn0.95Mg0.05]O2							0	65.54	7.044							
NaFe0.5Mn0.5O2					9.043			31.5	42.39							
NaMn0.5Ni0.5O2								0	30.86	0						
Na0.9[Mn0.4Fe0.5Ti0.1]O2					18.59			0	17.77					7.438		
NaMn1/3Fe1/3Ni1/3O2					13.56			4.493	0	271.6						
Na0.6Fe0.11Mn0.66Ni0.22O2					9.427			0	54.21	226.6						
NaMn0.3Fe0.4Ni0.3O2					12.48			4.066	9.513	0						
Na0.6Fe0.20Mn0.65Ni0.15O2					3.934			44.55	6.267	0						
Na0,6Ni0,22Al0,11Mn0,66O2	0							0	0	301.9						
LiFePO4					48.15	55.85					68.5					
Na3V2(PO4)3 [32]									0		23.2				69.814	
Na3V2(PO4)3 [33]									7.046		4.94				69.814	
Na3V2(PO4)3 [34]									6.976		4.94				69.814	
Na3V2(PO4)3 [35]									0		12				185.56	
Na3V2(PO4)3 [36]									6.976		7.99				189.93	
Na1.702Fe3(PO4)3					0				27.72		21.5					
Na4MnFe2(PO4)(P2O7)					0			0	65.53		9.86					
Na2MnPO4F/C				0.035				0	12.84		10.7					
Na2-δMn[Fe(CN)6]		0			0			0	7.471							
Na0.61Fe[Fe(CN)6]0.94		0			0											
GO@Na0.81Fe[Fe(CN)6]0.79					0											
Na2FeSiO4					0				0				43.19			
Na2MnSiO4								0	10.98				43.39			
NaFePO4					0				6.098		4.32					

Na4MnV(PO4)3 rGO									0	8.782		14.3				89.658	
Na3MnTi(PO4)3									0	6.962		15.1			12.88		
Na3MnTi(PO4)3									0	6.962		15.1			18.79		
Na3MnZr(PO4)3									0	6.359		4.6					0

Table 3: Numeric results for THP/kWh

	Al	C	Co	F	Fe	Li	Mg	Mn	Na	Ni	P	Pb	Si	Ti	V	Zr
NMC111			898.8			240.8		8.778		530.8						
NMC622			344.7			224.2		4.953		898.5						
NaMnO2								124.4	18.95							
Na0.67[Mn0.95Mg0.05]O2							0	144	15.48							
NaFe0.5Mn0.5O2					17.31			60.3	81.12							
NaMn0.5Ni0.5O2								0	85.12	0						
Na0.9[Mn0.4Fe0.5Ti0.1]O2					60.36			0	57.69					24.15		
NaMn1/3Fe1/3Ni1/3O2					49.3			16.34	0	987.8						
Na0.6Fe0.11Mn0.66Ni0.22O2					29.1			0	167.3	699.5						
NaMn0.3Fe0.4Ni0.3O2					32.01			10.43	24.39	0						
Na0.6Fe0.20Mn0.65Ni0.15O2					6.346			71.85	10.11	0						
Na0,6Ni0,22Al0,11Mn0,66O2	0							0	0	447.2						
LiFePO4					84.58	98.12					120					
Na3V2(PO4)3 [32]									0		62.1				187.01	
Na3V2(PO4)3 [33]									18.87		13.2				187.01	
Na3V2(PO4)3 [34]									18.69		13.2				187.01	
Na3V2(PO4)3 [35]									0		32.1				497.07	
Na3V2(PO4)3 [36]									18.69		21.4				508.77	
Na1.702Fe3(PO4)3					0				68.29		52.9					
Na4MnFe2(PO4)(P2O7)					0			0	158.7		23.9					
Na2MnPO4F/C				0.054				0	19.71		16.4					
Na2-δMn[Fe(CN)6]		0			0			0	15.25							
Na0.61Fe[Fe(CN)6]0.94		0			0											
GO@Na0.81Fe[Fe(CN)6]0.79					0											
Na2FeSiO4					0				0				59.65			
Na2MnSiO4								0	17.43				68.88			
NaFePO4					0				14.67		10.4					

Na4MnV(PO4)3 rGO									0	23.12		37.6				236	
Na3MnTi(PO4)3									0	13.76		29.9			25.45		
Na3MnTi(PO4)3									0	16.96		36.8			45.8		
Na3MnZr(PO4)3									0	15.8		11.4					0

4 LCA

All relevant assumptions for the LCA are provided in the following tables 2-7. The numeric results for HTox are provided in table 9 per kg and in table 10 per kWh.

Table 4: Overview of precursors and impact for LCA

	Aluminum nitrate nonahydrate	**Ammoniumeisen(II)-sulfat**	**Ammoniumhydrogenphosphat**	**Ammoniummetavanadat**	**Argon**	**cobalt(ii) sulfate heptahydrate**	**destilliertes Wasser**	**Diammonium dihydroxybis[lactato(2-)-O1,O2]titanate(2-)**	**Eisen(II)-oxalat**	**Eisen(II)-sulfat --> Heptahydrat**	**Eisen(III)-oxid**	**Ethanol, fossil**	**Ethanol, bio-based**	**Glucose**	**Grapheneoxid**	**Kaliumchlorid**
CAS	7784-27-2	7783-85-9	7722-76-1	7803-55-6	7440-37-1	10026-24-1	7732-18-5	65104-06-5	516-03-0	7782-63-0	1309-37-1	64-17-5	64-17-5	50-99-7		7447-40-7
			Diammonium phospha		H281, H280											
Formula	$Al(NO_3)_3 \cdot 9$	$(NH_4)_2Fe(S($	$(NH_4)H_2PO_4$	NH_4VO_3	Ar	$H_{14}CoO_{11}S$	H2O	$[CH_3CH(O-)CO_2NH_4]_2Ti(OH)_2$	FeC_2O_4	$FeSO_4$	Fe_2O_3	C_2H_5OH	C_2H_5OH	$C_6H_{12}O_6$		KCl
g/mol	375.13	392.14	115.03	116.98	40	281.1	18.02	294.08	179.89	278		46.07	46.07	180.156	12.01	74.55
g/mol (anhydrous)	212.98	284.05		116.98		154.996			143.91	151.9	159.7					
precursor 1	Al(OH)3	$FeSO_4$		0.5 V2O5				TiO_2	$FeSO_4$						synthetic graphite	
g/mol	77.98	151.9		181.88				80	151.9						12	
amount (kg/kg)	0.366138	0.534765		0.777398				0.27203482	1.055521						1	
Htox (CTUh/kg)	8.20E-08	7.79E-09		6.58E-06				1.54E-07	7.79E-09						3.77E-08	
precursor 2	3 HNO3	$(NH_4)_2SO_4$		(NH4)HCO3				missing	$C_2H_2O_4$						H2SO4	
g/mol	63	132.14		79.056					90.03							
amount (kg/kg)	0.887407	0.4652		0.675808					0.625599						1	
Htox (CTUh/kg)	9.50E-09	3.95E-08		2.89E-08					1.26E-07						3.94E-09	
Total																
Htox (CTUh/kg)	**2.18E-08**	**1.63E-08**	**2.51E-08**	**5.13E-06**	**1.33E-08**	**1.51E-06**		**4.19E-08**	**6.96E-08**	**4.26E-09**	**2.16E-08**	**1.02E-08**	**2.71E-07**	**4.55E-07**		**5.08E-08**
Htox (CTUh/kg), anhydro	**3.85E-08**	**2.25E-08**		**5.13E-06**		**2.73E-06**			**8.70E-08**	**7.79E-09**	**2.16E-08**				**4.16E-08**	

Table 5: Overview of precursors and impact for LCA

	Magnesiumacetat Tetrahydrat	Mangan(II)-acetat Tetrahydrat	Mangan(II)-nitrat	Mangan(II)-sulfat	Mangan(II)-sulfat Pentahydrat	Manganese(II) Oxalate Dihydrate	Manganese(II) sulfate monohydrate ACS	Manganoxalat	Manganoxid	Mangnesiumoxid	Natriumacetat für wasserhaltig Trihydrat cas 6131-90-4	Natriumcarbonat	Natriumchlorid	Natrium-dihydrogencarbonat	Natriumdiphosphat	Natriumferrocyanid	Natriumfluorid	Natriumhydroxid	Natriumnitrit
CAS	16674-78-5	6156-78-1	10377-66-9	10034-96-5	13465-27-5	6556-16-7	10034-96-5	640-67-5	1317-34-6	1309-48-4	127-09-3	497-19-8	7647-14-5	144-55-8	7722-88-5	13601-19-9	7681-49-4	1310-73-2	7632-00-0
														sodium bic	H319, H318,H302				
															sodium phosphate production				
Formula	$Mg(CH_3CO$	$Mn(CH_3CO$	$Mn(NO_3)_2$	$MnSO_4$	$MnSO4·5H$	$C_2H_6MnO_6$	H_2MnO_5S	$MnC_2O_4·2H$	MnO_2	MgO	$C_2H_3NaO_2$	Na_2CO_3	NaCl	$NaHCO_3$	$Na_4P_2O_7$	$Na_4Fe(CN)_6$	NaF	NaOH	$NaNO_2$
g/mol	214.46	245.09	178.95	243.093	243.093	178.99	169.02	142.96	87	40	136.08	105.988	58.44	84.007	265.9	303.91	42	40	69
g/mol (anhydrous)	142.394	173.027		151		142.956	151				82.03								
precursor 1	Mg(OH)2	MnSO4	MnSO4			MnSO4					NaOH					NaCN			
g/mol	58.3197	151	151			151					39.99					49.0072			
amount (kg/kg)	0.409566	0.872696	0.843811			0.843623					0.975009					0.967534			
Htox (CTUh/kg)	1.63E-08	2.12E-08	2.12E-08			2.12E-08					2.79E-08					4.04E-08			
precursor 2	2 CH3COOH	2 CH3CO2H	2 H N O 3			$C_2H_2O_4$					CH_3COOH					FeCl2			
g/mol	60.052	60.052	63			90.03					60.052					126.751			
amount (kg/kg)	0.843463	0.694134	0.704107			1.259548					0.732074					0.417068			
Htox (CTUh/kg)	3.19E-08	3.19E-08	9.50E-09			1.26E-07					3.19E-08					8.37E-09			
Total																			
Htox (CTUh/kg)	**2.23E-08**	**2.87E-08**	**2.46E-08**	**1.32E-08**	**1.32E-08**	**1.41E-07**	**1.89E-08**	**1.41E-07**	**8.62E-08**	**7.00E-08**	**3.05E-08**	**2.45E-08**	**1.31E-11**	**4.76E-08**	**1.64E-07**	**4.26E-08**	**1.10E-07**	**2.79E-08**	**4.89E-08**
Htox (CTUh/kg), anhydro	**3.36E-08**	**4.06E-08**		**2.12E-08**		**1.77E-07**	**2.12E-08**				**5.06E-08**								

Table 6: Overview of precursors and impact for LCA

	Natriumoxalat	Natriumperoxid	Nickel(II) acetate tetrahydrate	Nickel(II) sulfate hexahydrate	Nickel(II)-nitrat	Nickel(II)-Nitrat hexahydrat	Nickel(II)-sulfat	Nickeloxid	Oxalsäure	Phosphorsäure	Polyacrylsäure	Pyromellitsäure	Saccharose	Salzsäure	Schwefelsäure	Tetraethylenglycol	Tetraethylorthosilicat	Titan(IV)isopropoxid
CAS	62-76-0	1313-60-6	6018-89-9	10101-97-0	13138-45-9	13478-00-7	10101-97-0	1313-99-1	144-62-7	7664-38-2	#########	89-32-7		7647-01-0	7664-93-9	112-60-7	78-10-4	546-68-9
												Pyromellitic dianhydride (PMDA)						
Formula	$Na_2C_2O_4$	Na_2O_2	$Ni(OCOCH_3$	$NiSO_4 \cdot 6H_2$	$Ni(NO_3)_2$	$Ni(NO_3)_2 \cdot 6H_2$	$NiSO_4$	NiO	$C_2H_2O_4$	H_3PO_4	$(C_3H_4O_2)_n$	$C_{10}H_6O_8$	$C_{12}H_{22}O_{11}$	HCl	H_2SO_4	$C_8H_{18}O_5$	$SiC_8H_{20}O_4$	$Ti[OCH(CH_3$
g/mol	134	77.98	248.84	262.85	262.85	262.85	262.85	75		97.994	72.06	254.15	342.3	36.46	98	194.23	208.33	284.22
g/mol (anhydrous)			176.78	154.75	183		154.75		90.03									
precursor 1	NaOH		$NiSO_4$		$NiSO_4$			$NiSO_4$				Xylene					S i C l 4	TiO_2
g/mol	39.99		154.75		154.75			154.75				106.16					169.9	80
amount (kg/kg)	0.596866		0.875382		0.845628			2.063333				0.522133					0.815533	0.281472
Htox (CTUh/kg)	2.79E-08		4.54E-07		4.54E-07			4.54E-07				4.00E-09					2.56E-07	1.54E-07
precursor 2	$C_2H_2O_4$		2 CH3COOH		HNO3												ethanol	isopropano
g/mol	90.03		60.052		63.012												46.07	60.096
amount (kg/kg)	0.671866		0.482656		0.688656												0.884558	0.845767
Htox (CTUh/kg)	1.26E-07		3.19E-08		9.50E-09												1.02E-08	1.26E-08
Total																		
Htox (CTUh/kg)	**1.01E-07**	**6.15E-08**	**2.93E-07**	**2.67E-07**	**2.72E-07**	**2.71842E-07**	**2.67E-07**	**9.37E-07**	**1.26E-07**	**1.54E-08**	**1.06E-08**	**2.09E-09**	**4.55E-07**	**2.88E-07**	**3.94E-09**	**2.28E-08**	**2.18E-07**	**5.40E-08**
Htox (CTUh/kg), anhydro			**4.13E-07**	**4.54E-07**	**3.90E-07**		**4.54E-07**											

Table 7: Overview of precursors and impact for LCA

	Titanoxid	**Triethyl phosphate**	**Vanadium-Acetylacetonat**	**Vanadium pentoxid**	**Zirconium(IV) acetylacetonate**	**Zitronensäurelösung**
CAS	13463-67-7	78-40-0	3153-26-2	1314-62-1	17501-44-9	77-92-9
Formula	TiO_2	$(C_2H_5O)_3PO$	$C_{10}H_{14}O_5V$	V_2O_5	$C_{20}H_{28}O_8Zr$	$C_6H_8O_7 \cdot H_2O$
g/mol	80	182.15	265	181.88	487.66	192.12
g/mol (anhydrous)						
precursor 1		POCl3	V2O5		ZrO2	
g/mol		153.33	181.88		123.22	
amount (kg/kg)		0.841779	0.68634		0.252676	
Htox (CTUh/kg)		3.21E-07	6.58E-06		6.92E-08	
precursor 2	I	ethanol	isopropyl acetate		isopropyl acetate	
g/mol		46.07	102.133		102.133	
amount (kg/kg)		0.252923	1.734334		1.884914	
Htox (CTUh/kg)		1.02E-08	4.02E-08		4.02E-08	
Total						
Htox (CTUh/kg)	**1.54E-07**	**2.73E-07**	**4.59E-06**	**6.58E-06**	**9.33E-08**	**2.80E-07**
Htox (CTUh/kg), anhydro						

Table 8: Numeric results for Htox/kg

	Al	C	Co	F	Fe	Li	Mg	Mn	Na	Ni	P	Pb	Si	Ti	V	Zr
NMC111			1E-06			9E-08		7E-09		1E-07						
NMC622			6E-07			9E-08		4E-09		3E-07						
NaMnO2								7E-08	1E-08							
Na0.67[Mn0.95Mg0.05]O2							3E-09	7E-08	9E-09							
NaFe0.5Mn0.5O2					8E-09			3E-08	2E-08							
NaMn0.5Ni0.5O2								2E-08	3E-08	3E-07						
Na0.9[Mn0.4Fe0.5Ti0.1]O2					2E-08			3E-08	2E-08					1E-08		
NaMn1/3Fe1/3Ni1/3O2					2E-09			6E-09	6E-08	1E-07						
Na0.6Fe0.11Mn0.66Ni0.22O2					8E-10			2E-08	8E-09	1E-07						
NaMn0.3Fe0.4Ni0.3O2					1E-08			5E-09	1E-08	2E-07						
Na0.6Fe0.20Mn0.65Ni0.15O2					3E-09			5E-08	8E-09	1E-07						
Na0,6Ni0,22Al0,11Mn0,66O2	9E-09							2E-08	2E-08	2E-07						
LiFePO4					4E-09	1E-07					#####					
Na3V2(PO4)3 [32]									2E-08		0				5E-06	
Na3V2(PO4)3 [33]									9E-09		0				5E-06	
Na3V2(PO4)3 [34]									9E-09		0				5E-06	
Na3V2(PO4)3 [35]									3E-08		0				3E-06	
Na3V2(PO4)3 [36]									9E-09		0				3E-06	
Na1.702Fe3(PO4)3					1E-08				4E-09		0					
Na4MnFe2(PO4)(P2O7)					2E-08			4E-08	8E-08		0					
Na2MnPO4F/C				1E-09				3E-08	2E-08		0					
Na2-δMn[Fe(CN)6]					4E-08			1E-08	5E-12							
Na0.61Fe[Fe(CN)6]0.94					9E-08											
GO@Na0.81Fe[Fe(CN)6]0.79					8E-08											
Na2FeSiO4					5E-08				3E-08				2E-07			
Na2MnSiO4								4E-08	1E-08				2E-07			
NaFePO4					6E-08				7E-09		0					

Na4MnV(PO4)3 rGO								1E-08	1E-08		0				1E-06		
Na3MnTi(PO4)3								2E-08	9E-09		0			3E-08			
Na3MnTi(PO4)3								2E-08	9E-09		0			3E-08			
Na3MnZr(PO4)3								1E-08	8E-09		0					9E-08	

Table 9: Numeric results for HTox/kWh

		Al	C	Co	F	Fe	Li	Mg	Mn	Na	Ni	P	Pb	Si	Ti	V	Zr
NMC111				2E-06			2E-07		1E-08		2E-07						
NMC622				9E-07			1E-07		7E-09		4E-07						
NaMnO2									1E-07	2E-08							
Na0.67[Mn0.95Mg0.05]O2								6E-09	2E-07	2E-08							
NaFe0.5Mn0.5O2						1E-08			6E-08	4E-08							
NaMn0.5Ni0.5O2									5E-08	8E-08	9E-07						
Na0.9[Mn0.4Fe0.5Ti0.1]O2						5E-08			9E-08	7E-08					4E-08		
NaMn1/3Fe1/3Ni1/3O2						7E-09			2E-08	2E-07	4E-07						
Na0.6Fe0.11Mn0.66Ni0.22O2						2E-09			7E-08	2E-08	3E-07						
NaMn0.3Fe0.4Ni0.3O2						3E-08			1E-08	3E-08	5E-07						
Na0.6Fe0.20Mn0.65Ni0.15O2						5E-09			8E-08	1E-08	2E-07						
Na0,6Ni0,22Al0,11Mn0,66O2		1E-08							4E-08	2E-08	2E-07						
LiFePO4						7E-09	2E-07					0					
Na3V2(PO4)3 [32]										4E-08		0				1E-05	
Na3V2(PO4)3 [33]										2E-08		0				1E-05	
Na3V2(PO4)3 [34]										2E-08		0				1E-05	
Na3V2(PO4)3 [35]										7E-08		0				7E-06	
Na3V2(PO4)3 [36]										2E-08		0				7E-06	
Na1.702Fe3(PO4)3						3E-08				1E-08		0					
Na4MnFe2(PO4)(P2O7)						5E-08			9E-08	2E-07		0					
Na2MnPO4F/C					2E-09				5E-08	4E-08		0					
Na2-δMn[Fe(CN)6]						8E-08			3E-08	1E-11							
Na0.61Fe[Fe(CN)6]0.94						2E-07											
GO@Na0.81Fe[Fe(CN)6]0.79						2E-07											
Na2FeSiO4						7E-08				4E-08				3E-07			
Na2MnSiO4									6E-08	2E-08				4E-07			
NaFePO4						1E-07				2E-08		0					

Na4MnV(PO4)3 rGO								4E-08	3E-08		0				3E-06	
Na3MnTi(PO4)3								3E-08	2E-08		0			5E-08		
Na3MnTi(PO4)3								4E-08	2E-08		0			8E-08		
Na3MnZr(PO4)3								3E-08	2E-08		0					2E-07

5 Normalization, Weighted sum and hazard composite indicator

The indicators used for the hazard screening (THP) and those from the LCA (HTox) are rescaled to 1-3 using according to the minimum and maximum values provided in corresponding framework [33] to make them comparable as follows:

$$Cre, down = \frac{max_{re} - min_{re}}{max_{base} - min_{base}} * (x - min_{based}) + min_{new}$$ *Equation 1*

A simple weighted sum approach is used, with the performance of each alternative is calculated via Equation 10 [34]

$$A_i = \sum_{j=1}^{n} w_j a_{i,j} \; where \; i = 1, 2, 3, ...$$ *Equation 2*

Wj…..Attributed weights

Ai,j… considered alternative performance for one criterion

The composite indicator for THP and HTox is based on the simple average of the rescaled score of both sub-indicators and must be considered as purely qualitative to provide a first orientation for further assessments.

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