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Supplementary Information

A Preliminary Assessment of the 'Greenness' of Halide-Free Ionic Liquids- An MCDA based Approach

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1. Materials and Methods

1.1. Data collection and selection of halide-free ionic liquids

Firstly, a dataset of 193 halide- free ILs (HF-ILs) consisting of a combination of imidazolium, pyrrolidinium, pyridinium, piperidinium cations and carboxylic acid (acetic acid, propionic acid, butyric acid), alkyl sulfate (methyl, ethyl), sulfonate (methane, ethane) anions was prepared for analysis. Since the primary focus was on the development of halide free ILs for electroplating, CO_2 reduction, other electrochemical processes, alkyl groups for the cations were restricted upto butyl. Increasing the cationic chain length with higher alkyl group will increase the viscosity drastically and affect the overall performance. A combination of commercially available HF-ILs and HF-ILs designed through machine learning methods (artificial intelligence) were chosen for the analysis. The cation-anion combinations for HF-ILs are chosen considering the guidelines on selection of safer ILs by Costa et al.[1]. Since the safety data on the commercially available HF-ILs, designed HF-ILs are quite limited, safety information on the raw materials that are used for the synthesis are collected. The raw materials that are required for the synthesis of HF-ILs are taken from the literature [2–23]. Table S1 lists the details of the HF-ILs and their corresponding raw materials that have been used to synthesise the HF- ILs. As can be seen, few of the commercially available ILs are also used as the raw materials for the synthesis of HF- ILs. Unfortunately, the properties of HF-ILs are not fully defined, thus there is lot of missing information. Data for the missing information for the commercially available HF-ILs are filled with the data based on the raw materials that have been used for the synthesis of HF-ILs. Safety data sheets (SDS), research publications, The European Chemicals Agency (ECHA) register database[24], Pubchem[25], Chemspider[26] and the European Commission based projects were used as the sources to extract the information to the maximum possible. Additionally, few conventional organic solvents were also included in the list.

Table S1. Table lists the HF-ILs selected for analysis in this work and their corresponding raw materials.

S.No	Name of the Ionic Liquid	Raw Materials/Ionic Liquids
1	1-ethyl-3-methylimidazolium acetate	1-ethyl-3-methyl imidazolium acetate
2	1,3-dimethyl imidazolium acetate	1,3-dimethyl imidazolium chloride; acetic acid
3	1,3-diethyl imidazolium acetate (1-ethyl-3-ethyl imidazolium acetate)	formaldehyde; ethyl amine; glyoxal; acetic acid
4	1-propyl-3-methyl imidazolium acetate	1-propyl-3-methylimidazolium chloride; acetic acid; methanol; acetonitrile
5	1-butyl-3-methyl imidazolium acetate	1-butyl-3-methylimidazolium acetate
6	1-ethyl-2,3-dimethyl imidazolium acetate	1-methyl imidazole; chloroethane; acetic acid
7	1-butyl-2,3-dimethyl imidazolium acetate	1-methyl imidazole; chlorobutane; acetic acid
8	Pyridinium acetate	Pyridine; acetic acid
9	1-ethyl pyridinium acetate	1-ethyl pyridinium chloride; acetic acid
10	1-butyl pyridinium acetate	1-butyl pyridinium chloride; acetic acid
11	1-propyl-1-methyl piperidinium acetate	1-methyl piperidine; chloropropane; acetic acid
12	1-butyl-1-methyl piperidinium acetate	1-methyl piperidine; chlorobutane; sodium acetate
13	1-ethyl-3-methyl pyridinium acetate	1-ethyl-3-methyl pyridinium bromide;acetic acid
14	1-propyl-3-methyl pyridinium acetate	3-methyl pyridine (3-Picoline); chloropropane; acetic acid
15	1-butyl-2-methyl pyridinium acetate	1-butyl-2-methylpyridinium chloride; acetic acid
16	1-butyl-3-methyl pyridinium acetate	4-methyl pyridine (4-Picole);chlorobutane; acetic acid
17	1-butyl-4-methyl pyridinium acetate	1-butyl-4-methyl pyridinium chloride; acetic acid
18	1-methyl pyrrolidinium acetate	N-methyl pyrrolidine (1-methyl pyrrolidine); acetic acid
19	1-butyl-1-methyl pyrrolidinium acetate	N-methyl pyrrolidine (1-methyl pyrrolidine); chlorobutane;acetic acid
20	1,1,3,3-tetramethyl guanidinium acetate	1,1,3,3-tetramethyl guanidine; acetic acid
21	1-methyl imidazolium acetate	1-methyl imidazole; acetic acid
22	1-ethyl imidazolium acetate	1-ethyl imidazole; acetic acid
23	1-propyl imidazolium acetate	1-propyl imidazole; acetic acid
24	1-butyl imidazolium acetate	imidazole; chlorobutane; acetic acid
25	Choline acetate	cholinium hydroxide; acetic acid
26	1-ethyl-3-methyl imidazolium propionate	1-ethyl-3-methyl imidazolium propionate
27	1-butyl-3-methyl imidazolium propionate	1-methyl imidazole;chlorobutane; propionic acid
28	1,3-dimethyl imidazolium propionate (1-methyl-3-methyl imidazolium propionate)	1,3-dimethylimidazolium chloride; propionic acid
29	1,3-diethyl imidazolium propionate (1-ethyl-3-ethyl imidazolium propionate)	formaldehyde; ethyl amine; glyoxal;propionic acid
30	1,3-dibutyl imidazolium propionate (1-butyl-3-butyl imidazolium propionate)	1-butyl imidazole; chlorobutane; propionic acid
31	1-propyl-3-methyl imidazolium propionate	1-methyl imidazole; chloropropane; propionic acid
32	1-ethyl-2,3-dimethyl imidazolium propionate	1-methyl imidazole; chloroethane; propionic acid
33	1-butyl-2,3-dimethyl imidazolium propionate	1-methyl imidazole; chlorobutane; propionic acid
34	Pyridinium propionate	Pyridine; propionic acid
35	1-ethyl pyridinium propionate	1-ethyl pyridinium chloride; propionic acid
36	1-butyl pyridinium propionate	1-butyl pyridinium chloride; propionic acid
37	1-propyl-1-methyl piperidinium propionate	1-methyl piperidine; chloropropane; propionic acid
38	1-ethyl-3-methyl pyridinium propionate	1-ethyl-3-methyl pyridinium bromide; propionic acid

39	1-propyl-3-methyl pyridinium propionate	3-methyl pyridine (3-Picoline); chloropropane; propionic acid
40	1-butyl-3-methyl pyridinium propionate	3-methyl pyridine (3-Picoline); chlorobutane; propionic acid
41	1-butyl-4-methyl pyridinium propionate	1-butyl-4-methyl pyridinium chloride; propionic acid
42	1-butyl-1-methyl pyrrolidinium propionate	1-butyl-1-methyl pyrrolidinium chloride; propionic acid
43	1,1,3,3-tetramethyl guanidinium propionate	1,1,3,3-tetramethyl guanidine; propionic acid
44	Methyl propionate	chloromethane; propionic acid
45	Cholinium propionate	Cholinium hydroxide; propionic acid
46	1-methyl-2-pyrrolidinium propionate	1-methyl pyrrolidine; propionic acid
47	1-ethyl-3-methyl imidazolium butyrate	1-ethyl-3-methylimidazolium chloride;butyric acid
48	1,3-dimethyl imidazolium butyrate (1-methyl-3-methyl imidazolium butyrate)	1,3-dimethyl imidazolium chloride; butyric acid
49	1,3-diethyl imidazolium butyrate (1-ethyl-3-ethylimidazolium butyrate)	formaldehyde; ethyl amine; glyoxal; butyric acid
50	1-propyl-3-methyl imidazolium butyrate	1-propyl-3-methylimidazolium chloride; butyric acid
51	1-butyl-3-methyl imidazolium butyrate	1-Bbutyl-3-methylimidazolium chloride; butyric acid
52	1-ethyl-2,3-dimethyl imidazolium butyrate	1-methyl imidazole; chloroethane; butyric acid
53	1-butyl-2,3-dimethyl imidazolium butyrate	1-methyl imidazole; chlorobutane; butyric acid
54	1-ethyl pyridinium butyrate	1-ethyl pyridinium chloride; butyric acid
55	1-butyl pyridinium butyrate	1-butyl pyridinium chloride; butyric acid
56	1-propyl-1-methyl piperidinium butyrate	1-methylpiperidine; chloropropane; butyric acid
57	1-ethyl-3-methyl pyridinium butyrate	1-ethyl-3-methyl pyridinium bromide;butyric acid
58	1-propyl-3-methyl pyridinium butyrate	3-methyl pyridine (3-Picoline); chloropropane; acetic acid
59	1-butyl-3-methyl pyridinium butyrate	1-Butyl-3-methyl pyridinium chloride; butyric acid
60	1-butyl-4-methyl pyridinium butyrate	1-Butyl-4-methyl pyridinium chloride; butyric acid
61	1-butyl-1-methyl pyrrolidinium butyrate	1-Butyl-1-methyl pyrrolidinium chloride; butyric acid
62	1,1,3,3-tetramethyl guanidinium butyrate	1,1,3,3-tetramethyl guanidine; butyric acid
63	Cholinium butyrate	cholinium hydroxide; butyric acid
64	1-ethyl-3-methyl imidazolium bisulfate	1-ethyl-3-methylimidazolium bisulfate
65	1,3-dimethyl imidazolium bisulfate	formaldehyde;methyl amine;glyoxal; Sulfuric acid
66	1,3-diethyl imidazolium bisulfate	formaldehyde; ethyl amine; glyoxal; sulfuric acid
67	1-propyl-3-methyl imidazolium bisulfate	1-propyl-3-methyl imidazolium chloride; sodium bisulfate
68	1-butyl-3-methyl imidazolium bisulfate	1-butyl-3-methyl imidazolium bisulfate (1-butyl-3-methyl imidazolium hydrogen sulfate)
69	1-ethyl-2,3-dimethyl imidazolium bisulfate	1-methyl imidazole; chloroethane; sodium bisulfate
70	1-butyl-2,3-dimethyl imidazolium bisulfate	1-methyl imidazole; chlorobutane; sodium bisulfate
71	1-ethyl pyridinium bisulfate	1-butyl pyridinium chloride; Sodium bisulfate
72	1-butyl pyridinium bisulfate	1-ethyl pyridinium chloride; Sodium bisulfate
73	1-propyl-1-methyl piperidinium bisulfate	1-methyl piperidine; chloropropane; Sodium bisulfate
74	1-ethyl-3-methyl pyridinium bisulfate	1-ethyl-3-methyl pyridinium bromide; sodium bisulfate
75	1-propyl-3-methyl pyridinium bisulfate	1-methyl-3-propyl pyridinium bromide; Ssodium bisulfate
76	1-butyl-3-methyl pyridinium bisulfate	1-butyl-3-methylpyridinium chloride; sodium bisulfate
77	1-butyl-4-methyl pyridinium bisulfate	1-butyl-4-methyl pyridinium chloride; sodium bisulfate
78	1-butyl-1-methyl pyrrolidinium bisulfate	1-butyl-1-methyl pyrrolidinium chloride; sodium bisulfate
79	1,1,3,3-tetramethyl guanidinium bisulfate	1,1,3,3-Ttetramethyl guanidine; Sulfuric acid

80	1-methyl imidazolium hydrogen sulfate	1-methylimidazolium hydrogen sulfate
81	1-ethyl-3-methyl imidazolium methyl sulfate	1-ethyl-3-methyl imidazolium methyl sulfate
82	1,3-dimethyl imidazolium methyl sulfate (1-methyl-3-methylimidazolium methyl sulfate)	1-methyl imidazole; dimethyl sulfate
83	1,3-diethyl imidazolium methyl sulfate	1-ethyl imidazole; dimethyl sulfate
84	1-propyl-3-methyl imidazolium methyl sulfate	1-propyl imidazole; dimethyl sulfate
85	1-butyl-3-methyl imidazolium methyl sulfate	1-butyl imidazole; dimethyl sulfate
86	1-ethyl-2,3-dimethyl imidazolium methyl sulfate	1-ethyl imidazole; chloromethane; dimethyl sulfate
87	1-butyl-2,3-dimethyl imidazolium methyl sulfate	1-butyl imidazole; chloromethane; dimethyl sulfate
88	1-methyl pyridinium methyl sulfate	Pyridine; dimethyl sulfate
89	1,3-dimethyl pyridinium methyl sulfate	3-methyl pyridine (3-Picoline); dimethyl sulfate
90	2-ethyl-1-methyl pyridinium methyl sulfate	2-ethyl pyridine; dimethyl sulfate
91	1,1-dimethyl piperidinium methyl sulfate	1-methyl piperidine; dimethyl sulfate
92	1-ethyl-3-methyl pyridinium methyl sulfate	3-butyl pyridine; dimethyl sulfate
93	1-propyl-3-methyl pyridinium methyl sulfate	Pyridine; 1-chloropropane; dimethyl sulfate
94	1-butyl-3-methyl pyridinium methyl sulfate	3-butyl pyridine; dimethyl sulfate
95	1-butyl-4-methyl pyridinium methyl sulfate	1-butyl pyridinium chloride; dimethyl sulfate
96	1,1-dimethyl pyrrolidinium methyl sulfate	N-methylpyrrolidine (1-methyl pyrrolidine); dimethyl sulfate
97	1-ethyl-1-methyl pyrrolidinium methyl sulfate	N-ethylpyrrolidine(1-ethylpyrrolidine); dimethyl sulfate
98	1-propyl-1-methyl pyrrolidinium methyl sulfate	1-propyl pyrrolidine;dimethyl sulfate
99	1-butyl-1-methyl pyrrolidinium methyl sulfate	1-Butylpyrrolidine; dimethyl sulfate
100	1,2,3-trimethyl imidazolium methyl sulfate	1,2,3-Trimethyl imidazolium methyl sulfate
101	1-ethyl-3-methyl imidazolium ethyl sulfate	1-ethyl-3-methylimidazolium ethyl sulfate
102	1,3-dimethyl imidazolium ethyl sulfate (1-methyl-3-methylimidazolium ethyl sulfate)	1,3-dimethylimidazolium methyl sulfate(1-methyl-3-methylimidazolium methyl sulfate)
103	1,3-diethyl imidazolium ethyl sulfate (1-ethyl-3-ethylimidazolium ethyl sulfate)	1,3-diethyl imidazolium ethyl sulfate
105	1-ethyl-2,3-dimethyl imidazolium ethyl sulfate	1-ethyl-2,3-dimethyl imidazolium ethyl sulfate
107	1-ethyl pyridinium ethyl sulfate	Pyridine;diethyl sulfate
109	1,2-diethylpyridinium ethyl sulfate	2-ethyl pyridine;diethyl sulfate
110	1-ethyl-1-methyl piperidinium ethyl sulfate	1-methyl piperidine; dimethyl sulfate
112	1-ethyl-3-methyl pyridinium ethyl sulfate	3-methyl pyridine (3-Picoline); diethyl sulfate
113	1,1-dimethyl pyrrolidinium ethyl sulfate	N-ethylpyrrolidine(1-ethylpyrrolidine); dimethyl sulfate
114	1-ethyl-1-methyl pyrrolidinium ethyl sulfate	1-methyl pyrrolidine; diethyl sulfate
116	1-butyl-1-ethyl pyrrolidinium ethyl sulfate	1-butyl pyrrolidine; diethyl sulfate
118	2,2-diethyl-1,1,3,3-tetramethyl guanidinium ethyl sulfate	1,1,3,3-tetramethyl guanidine; diethyl sulfate; dichloro methane; sodium hydroxide
119	1-ethyl-3-methyl imidazolium methane sulfonate	1-ethyl-3-methyl imidazolium methane sulfonate
120	1,3-dimethyl imidazolium methane sulfonate (1-methyl-3-methylimidazolium methane sulfonate)	1,3-dimethyl imidazolium methanes ulfonate (1-methyl-3-methylimidazolium methane sulfonate)
121	1,3-diethyl imidazolium methane sulfonate (1-ethyl-3-ethyl imidazolium methane sulfonate)	formaldehyde; ethyl amine;glyoxal; methane sulfonic acid
122	1-propyl-3-methyl imidazolium methane sulfonate	1-propyl-3-methyl imidazolium chloride; methane sulfonic acid
123	1-butyl-3-methyl imidazolium methane sulfonate	1-butyl-3-methyl imidazolium methane sulfonate

124	1-ethyl-2,3-dimethyl imidazolium methane sulfonate	1-ethyl-2,3-dimethyl imidazolium chloride;methane sulfonic acid
125	1-butyl-2,3-dimethyl imidazolium methane sulfonate	1-butyl-2,3-dimethyl imidazolium chloride; methane sulfonic acid
126	1-propyl-1-methyl piperidinium methane sulfonate	1-methyl piperidine; chloropropane;methane sulfonic acid
127	1-ethyl-3-methyl pyridinium methane sulfonate	1-ethyl-3-methyl pyridinium bromide; methane sulfonic acid
128	1-propyl-3-methyl pyridinium methane sulfonate	1-methyl-3-propyl pyridinium bromide; methane sulfonic acid
129	1-butyl-2-methyl pyridinium methane sulfonate	1-butyl-2-methyl pyridinium chloride; methane sulfonic acid
130	1-butyl-3-methyl pyridinium methane sulfonate	1-butyl-3-methyl pyridinium chloride; methane sulfonic acid
131	1-butyl-4-methyl pyridinium methane sulfonate	1-butyl-4-methyl pyridinium chloride;methane sulfonic acid
132	1-propyl-1-methyl pyrrolidinium methane sulfonate	N-methyl pyrrolidine (1-methyl pyrrolidine); chloropropane; methane sulfonic acid
133	1-butyl-1-methyl pyrrolidinium methane sulfonate	1-butyl-1-methyl pyrrolidinium chloride; methane sulfonic acid
134	1-butyl-1-ethyl pyrrolidinium methane sulfonate	N-ethylpyrrolidine (1-ethyl pyrrolidine); chloropropane; methane sulfonic acid
135	1,1,3,3-tetramethyl guanidinium methane sulfonate	1,1,3,3-tetramethyl guanidine; methane sulfonic acid
136	1-ethyl-3-methyl imidazolium ethane sulfonate	1-ethyl-3-methyl imidazolium ethane sulfonate
137	1,3-dimethyl imidazolium (1-methyl-3-methyl imidazolium) ethane sulfonate	1,3-dimethyl imidazolium chloride; ethane sulfonic acid
138	1,3-diethyl imidazolium ethyl sulfate (1-ethyl-3-ethylimidazolium) ethane sulfonate	formaldehyde; ethyl amine; glyoxal; ethane sulfonic acid
139	1-propyl-3-methylimidazolium ethane sulfonate	1-propyl-3-methyl imidazolium chloride; ethane sulfonic acid
140	1-butyl-3-methyl imidazolium ethane sulfonate	1-butyl-3-methyl imidazolium chloride; ethane sulfonic acid
141	1-ethyl-2,3-dimethyl imidazolium ethane sulfonate	1-ethyl-2,3-dimethylimidazolium ethane sulfonate
142	1-butyl-2,3-dimethyl imidazolium ethane sulfonate	1-butyl-2,3-dimethylimidazolium chloride; ethane sulfonic acid
143	1-butyl pyridinium ethane sulfonate	1-butyl pyridinium chloride; ethane sulfonic acid
144	1-propyl-1-methyl piperidinium ethane sulfonate	1-methyl piperidine; chloropropane; ethane sulfonic acid
145	1-ethyl-3-methyl pyridinium ethane sulfonate	1-ethyl-3-methyl pyridinium bromide; ethane sulfonic acid
146	1-propyl-3-methyl pyridinium ethane sulfonate	1-methyl-3-propyl pyridinium bromide; ethane sulfonic acid
147	1-butyl-2-methyl pyridinium ethane sulfonate	1-butyl-2-methyl pyridinium chloride;ethane sulfonic acid
148	1-butyl-3-methyl pyridinium ethane sulfonate	1-butyl-3-methyl pyridinium chloride; ethane sulfonic acid
149	1-butyl-4-methyl pyridinium ethane sulfonate	1-butyl-4-methyl pyridinium chloride; ethane sulfonic acid
150	1-propyl-1-methyl pyrrolidinium ethane sulfonate	N-methyl pyrrolidine (1-methyl pyrrolidine); chloropropane; ethane sulfonic acid
151	1-butyl-1-methyl pyrrolidinium ethane sulfonate	1-butyl-1-methyl pyrrolidinium chloride;ethane sulfonic acid
152	1,1,3,3-tetramethyl guanidinium ethane sulfonate	1,1,3,3-tetramethyl guanidine; ethane sulfonic acid

153	2-hydroxyethyl ammonium propionate	ethanolamine (2-aminoethanol); propionic acid
154	1-propyl-2,3-dimethyl imidazolium acetate	1,3-dimethylimidazolium chloride; chloropropane; acetic acid
155	1-ethyl-2-butyl pyridinium acetate	2-ethyl pyridine; chlorobutane; acetic acid
156	1,1-dimethyl pyrrolidinium acetate	N-methyl pyrrolidine (1-methyl pyrrolidine); chloromethane; acetic acid
157	1-butyl-1-ethyl pyrrolidinium acetate	N-ethylpyrrolidine (1-ethyl pyrrolidine); chlorobutane; acetic acid
158	1-propyl-2,3-dimethyl imidazolium propionate	1,3-dimethyl imidazolium chloride; chloropropane; propionic acid
159	1-methyl-3-propyl pyridinium propionate	1-methyl-3-propyl pyridinium bromide; propionic acid
160	1-butyl-2-methyl pyridinium propionate	2-methyl pyridine; chlorobutane; propionic acid
161	1,1-dimethyl pyrrolidinium propionate	N-methyl pyrrolidine (1-methyl pyrrolidine); chloromethane; propionic acid
162	1-propyl-1-methyl pyrrolidinium propionate	N-methyl pyrrolidine (1-methyl pyrrolidine); chloropropane; propionic acid
163	1-butyl-1-ethyl pyrrolidinium propionate	N-ethyl pyrrolidine (1-ethyl pyrrolidine); chlorobutane; propionic acid
164	1-propyl-2,3-dimethyl imidazolium butyrate	1,3-dimethyl imidazolium chloride; chloropropane; butyric acid
165	1-methyl-3-propyl pyridinium butyrate	1-methyl-3-propyl pyridinium bromide; butyric acid
166	1-butyl-2-methyl pyridinium butyrate	2-methylpyridine; chlorobutane; butyric acid
167	1-ethyl-2-butyl pyridinium butyrate	2-ethyl pyridine; chlorobutane; butyric acid
168	1,1-dimethyl pyrrolidinium butyrate	N-methyl pyrrolidine (1-methyl pyrrolidine); chloromethane; butyric acid
169	1-butyl-1-ethyl pyrrolidinium butyrate	N-ethylpyrrolidine(1-ethylpyrrolidine); chlorobutane; butyric acid
170	1-methyl-3-propyl imidazolium bisulfate	1-propyl-3-methyl imidazolium chloride; sodium bisulfate
171	1-propyl-2,3-dimethyl imidazolium bisulfate	1,3-dimethyl imidazolium chloride; chloropropane; sodium bisulfate
172	1-methyl-3-propyl pyridinium bisulfate	1-methyl-3-propyl pyridinium bromide; sodium bisulfate
173	1-butyl-2-methyl pyridinium bisulfate	2-methylpyridine; chlorobutane; sodium bisulfate
174	1-ethyl-2-butyl pyridinium bisulfate	2-ethyl pyridine; chlorobutane; sodium bisulfate
175	1,1-dimethyl pyrrolidinium bisulfate	N-methyl pyrrolidine (1-methyl pyrrolidine); chloromethane; sulfuric acid
176	1-propyl-1-methyl pyrrolidinium bisulfate	N-methyl pyrrolidine (1-methyl pyrrolidine); chloropropane; sulfuric acid
177	1-propyl-2,3-dimethyl imidazolium methyl sulfate	1-propyl-3-methyl imidazolium chloride; dimethyl sulfate
178	1-propyl-2,3-dimethyl imidazolium ethyl sulfate	1-propyl-3-methyl imidazolium chloride; diethyl sulfate
183	1-propyl-2,3-dimethyl imidazolium methane sulfonate	1,3-dimethyl imidazolium chloride; chloropropane; methane sulfonic acid
184	1-ethylpyridinium methane sulfonate	1-ethyl pyridinium chloride; methane sulfonic acid
185	1-methyl-3-propyl pyridinium methane sulfonate	1-methyl-3-propyl pyridinium bromide; methane sulfonic acid
186	1-ethyl-2-butyl pyridinium methane sulfonate	2-ethyl pyridine; chlorobutane; ethane sulfonic acid
187	1,1-dimethyl pyrrolidinium methane sulfonate	N-methyl pyrrolidine (1-methylpyrrolidine); chloromethane; methane sulfonic acid
188	1-propyl-2,3-dimethyl imidazolium ethane sulfonate	1,3-dimethyl imidazolium chloride; chloro propane; ethane sulfonic acid

189	1-ethyl pyridinium ethane sulfonate	1-ethyl pyridinium chloride; ethane sulfonic acid
190	1-methyl-3-propyl pyridinium ethane sulfonate	1-methyl-3-propyl pyridinium bromide; ethane sulfonic acid
191	1-ethyl-2-butyl pyridinium ethane sulfonate	2-ethyl pyridine; chlorobutane; ethane sulfonic acid
192	1-butyl-1-ethyl pyrrolidinium ethane sulfonate	N-ethylpyrrolidine(1-ethylpyrrolidine); chlorobutane; ethane sulfonic acid
193	1-butyl-1-ethyl pyrrolidinium methane sulfonate	N-ethyl pyrrolidine(1-ethylpyrrolidine); chlorobutane;methane sulfonic acid

The criteria and the relevant source of information that was chosen for the study are shown in Table S2. To collect the information on criteria such as signal wording, hazard statements, precautionary statements, carcinogenicity, special hazards arising from the substance or mixture/hazardous decomposition products, safety data sheets (SDS) were referred from the following list of companies to collect the information

- Sigma Aldrich
- Acros Organics
- Alfa Aesar
- BASF
- Carl Roth
- ChemSrc
- Merck
- Santa Cruz Biotechnology Inc.
- Sisco Research Laboratories Pvt. Ltd. (SRL)
- Solvionic
- Tokyo Chemical Industry (TCI) Chemicals
- Thermo Fisher Scientific
- Proionic
- Iolitec

Values for Octanol-water coefficient and biodegradation parameters as well as Toxicity towards different organisms: *Daphnia Magna*, *algae*, *fish, rodents ingestion (oral route)* are taken from SDS collected from the list of companies mentioned above, scientific papers and additionally from European Chemical Agency (ECHA) database register[24], PubChem[25], Chemspider[26]. For The Technique for Order of Preferentiality by Similarity to Ideal Solution (TOPSIS) analysis, numerical values are required. Therefore the collected information have been transformed, into numerical values adopting the procedure reported by Marta et al.[27,28]. Since the data availability for designed and other commercial HF-ILs from company databases like Sigma-Aldrich, Solvionic, Iolitec, are limited, most information for analysis in our work are collected through the Safety Data Sheets (SDS) available from those companies as mentioned above.

Table S2. Criteria, parameters describing the ionic liquids along with their weighting factors

Criterion	Description	Source	Weightage
H-statements	Hazard statements are transformed numerically into points	Safety data sheets, papers, ECHA database, Pubchem, Chemspider	0.06
P-statements	Precaution statements are transformed numerically into points	Safety data sheets, papers, ECHA database, Pubchem, Chemspider	0.06
Signal wording	Descriptions are transformed numerically into points	Safety data sheets,	0.02

		papers, ECHA database, Pubchem, Chemspider	
Hazardous decomposition products	Descriptions related to the combustion of hazardous products are transformed numerically into points	Safety data sheets, papers, ECHA database, Pubchem, Chemspider	0.02
Biodegradability	28 days degradation test expressed in %	Safety data sheets, papers, ECHA database, Pubchem, Chemspider	0.1
Toxicity Daphnia magna	48 h/24 h test data was collected based on the availability	Safety data sheets, papers, ECHA database, Pubchem, Chemspider	0.13
Toxicity algae	96 h/72 h test data was collected based on the availability	Safety data sheets, papers, ECHA database, Pubchem, Chemspider	0.13
Toxicity fish	96 h/48 h test data was collected based on the availability	Safety data sheets, papers, ECHA database, Pubchem, Chemspider	0.13
Toxicity rodents via ingestion	Test data rodents (rats or other similar preferable organism) body mass	Safety data sheets, papers, ECHA database, Pubchem, Chemspider	0.13
Flash point	Expressed in K	Safety data sheets, papers, ECHA database, Pubchem, Chemspider	0.04
Partition coefficient, Log P_{ow}	Dimensionless	Safety data sheets, papers, ECHA database, Pubchem, Chemspider	0.04
Vapor pressure	Expressed in hPa at 25 °C	Safety data sheets, papers, ECHA database, Pubchem, Chemspider	0.06
pH	Dimensionless	Safety data sheets, , ECHA database, Pubchem, Chemspider	0.04
Carcinogenity	Human carcinogenicity classification based on IARC are translated into numbers – group 1 (5), group 2A (4) and group 2B (3.5)	Safety data sheets, papers, ECHA database, Pubchem, Chemspider	0.04

1.2. Multi-criteria decision analysis (MCDA)-TOPSIS

Multicriteria decision analysis (MCDA) is a collection of methodologies aimed at identifying the most favourable alternative while ranking all the remaining ones [29,30]. MCDA helps to integrate the results of multiple evaluation criteria into a single, easily interpreted number - one for each alternative. It's especially useful when the assessment criteria are at odds with one another. To put it in another way, MCDA allows one to prioritise all the alternatives (such as ILs) based on the ranking through TOPSIS methodology. Hwang and Yoon [31] developed TOPSIS algorithm which helps to identify the best alternative by transforming all the criteria into a numerical matrix, calculate the shortest

and longest distance from the ideal and non-ideal solution. The key advantage with TOPSIS method is that, it allows to rank all the alternatives by combining different criteria and obtaining a single value, which is based on the similarity to the ideal solution ranging from 0 to 1. "0" infers to a completely non-ideal (or negative ideal) option, indicating that it is characterised by the worst values for each and every criterion, farthest distance from the completely ideal (or positive ideal) solution. On the contrary, "1" indicates that an ideal solution has been identified, indicating that the best values have been obtained for all the criteria and, has attained the shortest distance from the completely ideal solution. In order to apply this methodology, the criteria that has been selected to evaluate the greenness of ILs has to be transformed into numerical values. Prior to the analysis, the information collected on different criteria from sources (as mentioned above) for different raw materials was transformed into numerical values by adopting the methodology proposed by Marta et al.[27,28]. The numerical values are represented as a *n x m* matrix consisting of n raw materials (=74*)* against *m* criteria (=14).

One of the primary benefits with TOPSIS is that its capability to combine numerous different criteria into a single score and obtain full ranking, and assigning the ranking based on the value of similarity to ideal solution. In this way, the collected information that is transformed into numerical, is converted into a single score for each alternative through TOPSIS. The ordering of the alternatives is ranked based on the alternative's calculated distance to the completely ideal solution (value of similarity to the ideal solution).

1.2.1. TOPSIS Algorithm

The input data for TOPSIS analysis is the matrix consisting of *n(=74)* raw materials as rows and *m(=14)* criteria as columns, which are transformed into numerical data points. The algorithm is represented in 6 steps as follows:

1. Construction of normalised decision matrix

$$r_{ij} = x_{ij} \div \sqrt{\sum x_{ij}^2}, \quad \text{i} = 1, 2, \dots, \text{m and j} = 1, 2, \dots, \text{n} \qquad (1)$$

- Where x_{ij} and r_{ij} are original and normalised scores in decision matrix, respectively (subscripts i, j represents the row index and column index of the respective numerical data point)

2. Construction of the weighted normalised decision matrix

$$v_{ij} = r_{ij} \times w_j, \quad \text{i} = 1, 2, \dots, \text{m and j} = 1, 2, .., \text{n} \qquad (2)$$

Where w_j is the weight of the criterion and $\sum_{j=1}^{n} w_j = 1$

3. Determination of positive ideal (A^*) and negative ideal (A^-) solutions

$$A^* = \{(max_i v_{ij} | j \in C_b), (min_i v_{ij} | j \in C_c)\} = \{v_i^* | j = 1, 2, \dots, m\} \quad (3)$$

$$A^- = \{(min_i v_{ij} | j \in C_b), (max_i v_{ij} | j \in C_c)\} = \{v_j^* | j = 1, 2, \dots, m\} \quad (4)$$

4. Calculation of the separation measures for each alternative

$$S_i^* = \sqrt{\sum_{j=1}^{m} \left(v_{ij} - v_j^*\right)^2} \; \text{j} = 1, 2, \dots, \text{m} \quad (5)$$

$$S_i^- = \sqrt{\sum_{j=1}^{m} \left(v_{ij} - v_j^-\right)^2} \; \text{j} = 1, 2, \dots, \text{m} \quad (6)$$

5. Calculation of the relative closeness to the ideal solution

$$C_i^* = \frac{S_i^-}{S_i^* + S_i^-}, \quad \mathrm{i} = 1, 2, \ldots, \mathrm{m} \text{ and } 0 < \mathrm{C_i^*} < 1 \quad (7)$$

6. Arrangement of scenarios in order of closest to ideal ("1") to farthest from ideal ("0")–creation of a ranking
The alternative with $\mathrm{C_i^*}$ closest to 1 is the best preference among the possible options.

TOPSIS algorithm presented above is the simplest possible representation and detailed information explaining the fundamentals can be found elsewhere [31–33]. Calculations performed stepwise as per TOPSIS algorithm were carried out using Microsoft Excel program (MS-Excel 2016) adopting the methodology developed by Hwang et al. [31]. Prior to estimation of the quantifiable responses for the HF-ILs, the relativeness closeness to the ideal solutions for the raw materials was evaluated followed by sensitivity analysis at ±10 %. The results are shown in Table S3. Based on the data set of raw materials, it is observed that toxicity, hazard and precautionary statements are observed as the major influencing factors. Therefore, these values were changed randomly and the newly calculated relativeness closeness to ideal solutions (representing the sensitivity changes) along with their relative ranking differences are shown in Table S3. As can be seen from the table, it is evident that there are no significant differences in the overall ranking indicating that the ranking results are safely reliable and considered to be accurate. The HF-ILs mixture that could be synthesized from these basic ingredients(as mentioned in Table S1) are expected to function similarly, guided by the same mechanism/mode of action, and differ solely in potencies, according to general principles of mixture toxicology [34].

Considering such scenario, effects can be calculated simply from the sum of doses/concentrations, adjusted for relative toxicity (dose/concentration addition) for mixtures of similar acting substances (such as HF-ILs).

$$E(Cmix) = \sum_{i=1}^{n} aE(Ci) \quad (8)$$

where $E(C_{mix})$ is combined effect at the equimolar mixture concentration of raw materials (C_{mix}), and $E(C_i)$ is the similarity to ideal solution (calculated for different raw materials with TOPSIS) of individual mixture component (i) applied at the concentration (Ci). In principle, doses or concentrations of the single components are added after being multiplied by a scaling factor "a" that accounts for differences in the potency of the individual substances. In our analysis, we have assumed a=1 considering an equimolar ratios of the raw materials for the preparation of HF-ILs.

Values of similarity to the ideal solution obtained by evaluating the combined greenness effect from equation (8) are represented as $E(C_{mix})$ in Table S4.

Table S3. Table showing the results of TOPSIS analysis for raw materials. For the sake of brevity, the relative closeness to the ideal solution, ranking, ranking difference for ± 10% sensitivity changes are represented separately.

S.No	Raw Materials	Ci*	Ranking	$C_{i^*,\pm10\%}$	Ranking	Rank Difference ($C_{i^*,\pm10\%}$,Ci*)
1	1,1,3,3-tetramethylguanidine	0.62834	1	0.62574	1	0
2	1-butyl imidazole	0.20584	2	0.20861	2	0

3	1-butyl-2,3-dimethylimidazolium chloride	0.20399	3	0.20180	3	0
4	1-butyl-3-methylimidazolium bromide	0.17182	4	0.16376	5	1
5	1-butyl-3-methylimidazolium chloride	0.17165	5	0.17403	4	-1
6	1-butyl-3-methylpyridinium chloride	0.15802	6	0.15974	6	0
7	1-butylpyrrolidine	0.15299	7	0.15313	7	0
8	1-chloropropane	0.13865	8	0.13859	8	0
9	1-ethyl imidazole	0.13534	9	0.13224	9	0
10	1-ethyl pyridinium chloride	0.13088	10	0.13083	10	0
11	1-ethyl-3-methylimidazolium bromide	0.12122	11	0.12090	11	0
12	1-ethyl-3-methylimidazolium chloride	0.12095	12	0.12084	12	0
13	1-ethyl-3-methyl pyridinium bromide	0.11732	13	0.11736	13	0
14	1-methyl imidazole	0.11682	14	0.11633	14	0
15	1-methyl piperidine	0.11622	15	0.11037	23	8
16	1-Methyl pyrrolidine	0.11619	16	0.11616	15	-1
17	1-Propyl imidazole	0.11539	17	0.11528	16	-1
18	1-propyl-3-methylimidazolium chloride	0.11466	18	0.11431	18	0
19	1-propyl pyrrolidine	0.11425	19	0.11410	19	0
20	2-ethyl pyridine	0.11393	20	0.11490	17	-3
21	2-methyl imidazole	0.11343	21	0.11273	21	0
22	3-butyl pyridine	0.11330	22	0.11393	20	-2
23	3-methyl pyridine (3-Picoline)	0.11319	23	0.10922	26	3
24	Acetic Acid	0.11191	24	0.11166	22	-2
25	Acetonitrile	0.10998	25	0.11002	24	-1
26	Butyric acid	0.10982	26	0.10934	25	-1
27	chlorobutane	0.10899	27	0.10895	27	0
28	chloroethane	0.10828	28	0.10772	29	1
29	chloromethane	0.10826	29	0.10815	28	-1
30	cholinium hydroxide	0.10773	30	0.10764	30	0
31	dichloro methane	0.10728	31	0.10727	32	1
32	Diethyl sulfate	0.10711	32	0.10634	33	1
33	Dimethyl sulfate	0.10636	33	0.10619	34	1
34	Ethane sulfonic acid	0.10621	34	0.10734	31	-3
35	Ethanol	0.10621	35	0.10595	36	1
36	Ethanolamine (2-aminoethanol)	0.10609	36	0.10602	35	-1
37	Ethyl acetate	0.10516	37	0.10463	38	1
38	Ethyl amine	0.10492	38	0.10465	37	-1
39	Formaldehyde	0.10270	39	0.10303	39	0
40	Glyoxal	0.10246	40	0.10257	40	0
41	Imidazole	0.09777	41	0.09765	42	1

42	Methane sulfonic acid	0.09746	42	0.09771	41	-1
43	Methanol	0.09710	43	0.09699	43	0
44	Methyl amine	0.09512	44	0.09438	45	1
45	Methyl Propionate	0.09453	45	0.09442	44	-1
46	N-butyl amine (1- Amino butane, n-Butylamine)	0.09334	46	0.09316	48	2
47	N-ethylpyrrolidine(1-ethylpyrrolidine)	0.09333	47	0.09321	47	0
48	1-methylpiperidine	0.09324	48	0.09356	46	-2
49	N-methylpyrrolidine (1-methylpyrrolidine)	0.09241	49	0.09266	49	0
50	Propionic acid	0.09110	50	0.09098	50	0
51	Propyl amine (1-Aminopropane)	0.09028	51	0.09017	51	0
52	Pyridine	0.09026	52	0.09015	52	0
53	Silver acetate	0.09025	53	0.09014	53	0
54	Sodium acetate	0.08993	54	0.08985	54	0
55	Sodium bisulfate	0.08906	55	0.08897	55	0
56	Sodium ethoxide (Sodium ethylate)	0.08861	56	0.08851	56	0
57	Sodium Hydroxide	0.08738	57	0.08738	57	0
58	Sulfuric acid	0.08644	58	0.08631	58	0
59	Toluene	0.08251	59	0.08274	59	0
60	1-butyl pyridinium chloride	0.08245	60	0.08195	62	2
61	1-ethyl-2,3-dimethylimidazolium chloride	0.08208	61	0.08200	61	0
62	1-methyl-3-propylpyridinium bromide	0.08206	62	0.08250	60	-2
63	Sodium butyrate	0.08120	63	0.07817	64	1
64	1-butyl-2-methylpyridinium chloride	0.08087	64	0.08099	63	-1
65	1-butyl-1-methylpyrrolidinium chloride	0.07818	65	0.07683	65	0
66	1-Butyl-4-methylpyridinium chloride	0.07508	66	0.07496	66	0
67	1,3-dimethylimidazolium chloride	0.07480	67	0.074714 2	67	0
68	1,2-dimethylimidazole	0.07193	68	0.07203	68	0
69	Butanol	0.06912	69	0.06907	69	0
70	Bromoethane	0.06276	70	0.06264	70	0
71	4-methyl pyridine (4-Picole)	0.06208	71	0.06201	71	0
72	2-methylpyridine	0.05897	72	0.05919	72	0
73	1-Propanol	0.05019	73	0.05011	73	0
74	Pyrrolidine	0.04802	74	0.04802	74	0

Table S4. Overall ranking of the halide free ILs

Ranking	Name of the Ionic Liquid	Abbrevation	Similarity to the ideal solution value, E(C_{mix})
1	methanol	[MeOH]	0.62834
2	1,3-diethyl imidazolium acetate	[EE'Im][OAc]	0.46447
3	1-ethyl-2-butyl pyridinium bisulfate	[E2BPyr][HSO_4]	0.46441
4	1,3-diethyl imidazolium propionate	[EE'Im][C_2COO}	0.46025
5	1-propyl-1-methyl piperidinium bisulfate	[PMPip][HSO_4]	0.45638
6	1,3-diethyl imidazolium butyrate	[EE'Im][C_3COO]	0.45439
7	1,3-dimethyl imidazolium bisulfate	[MM'Im][HSO_4]	0.44969
8	1-propyl-2,3-dimethyl imidazolium bisulfate	[PMM'Im][HSO_4]	0.44879
9	1,3-diethyl imidazolium bisulfate	[EE'Im][HSO_4]	0.42599
10	2,2-diethyl-1,1,3,3-tetramethyl guanidinium ethyl sulfate	[EE'TMG][$EtSO_4$]	0.41882
11	1,3-diethyl imidazolium methane sulfonate	[EE'Im][CH_3SO_3]	0.41720
12	1,3-diethyl imidazolium ethane sulfonate	[EE'Im][$C_2H_5SO_3$]	0.41503
13	1-butyl-1-ethyl pyrrolidinium acetate	[BEPyrl][OAc]	0.41328
14	1-butyl-1-ethyl pyrrolidinium propionate	[BEPyrl][C_2COO]	0.40906
15	1-butyl-1-ethyl pyrrolidinium methane sulfonate	[BEPyrl][CH_3SO_3]	0.40903
16	1-ethyl-2,3-dimethyl imidazolium bisulfate	[EMM'Im][HSO_4]	0.40766
17	1-butyl-1-ethyl pyrrolidinium butyrate	[BEPyrl][C_3COO]	0.40320
18	1-butyl-2,3-dimethyl imidazolium bisulfate	[BMM'Im][HSO_4]	0.40032
19	1-butyl-2,3-dimethyl imidazolium methyl sulfate	[BMM'Im][$MeSO_4$]	0.39949
20	1-ethyl-2,3-dimethyl imidazolium methyl sulfate	[EMM'Im][$MeSO_4$]	0.38581
21	1-butyl-2-methyl pyridinium bisulfate	[B2MPyr][HSO_4]	0.38369
22	1-ethyl-2-butyl pyridinium acetate	[E2BPyr][OAc]	0.37927
23	1-propyl-1-methyl piperidinium acetate	[PMPip][OAc]	0.37015
24	1-ethyl-2-butyl pyridinium butyrate	[E2BPyr][C_3COO]	0.36918
25	1-propyl-1-methyl piperidinium propionate	[PMPip][C_2COO]	0.36701
26	1-butyl-1-ethyl pyrrolidinium methane sulfonate	[BEPyrl][CH_3SO_3]	0.36601
27	1-butyl-1-ethyl pyrrolidinium ethane sulfonate	[BEPyrl][$C_2H_5SO_3$]	0.36384
28	1-propyl-2,3-dimethyl imidazolium acetate	[PMM'Im][oAc]	0.36364
29	1-propyl-1-methyl piperidinium butyrate	[PMPip][C_3COO]	0.36007
30	1-propyl-2,3-dimethyl imidazolium propionate	[PMM'Im][C_2COO]	0.35942
31	Choline acetate	[Ch][OAc]	0.35756
32	ethanol	[EtOH]	0.35613
33	1-propyl-3-methyl imidazolium propionate	[PMIm][C_2COO]	0.35396
34	1-propyl-2,3-dimethyl imidazolium butyrate	[PMM'Im][C_3COO]	0.35356
35	Choline propionate	[Ch][C_2COO]	0.35333
36	1,1-dimethyl pyrrolidinium acetate	[MM'Pyrl][oAc]	0.35101
37	Choline butyrate	[Ch][C_3COO]	0.34748
38	1,1-dimethyl pyrrolidinium propionate	[MM'Pyrl][C_2COO]	0.34679
39	1-propyl-3-methyl pyridinium acetate	[PMPyr][OAc]	0.34379
39	1-propyl-3-methyl pyridinium butyrate	[P3MPyr][C_3COO]	0.34379

41	1,1-dimethyl pyrrolidinium butyrate	[MM'Pyr][C_3COO]	0.34093
42	1-propyl-3-methyl pyridinium propionate	[PMPyr][C_2COO]	0.33957
43	1-propyl-1-methyl pyrrolidinium propionate	[PMPyrl][C_2COO]	0.33648
44	1-ethyl-2-butyl pyridinium methane sulfonate	[E2BPyr][CH_3SO_3]	0.32982
44	1-ethyl-2-butyl pyridinium ethane sulfonate	[E2BPyr][$C_2H_5SO_3$]	0.32982
46	1-propyl-3-methyl pyridinium methyl sulfate	[PMPyr][$MeSO_4$]	0.32609
47	1,3-dibutyl imidazolium propionate	[BB'Im][C_2COO]	0.32516
48	1-propyl-1-methyl piperidinium methane sulfonate	[PMPip][CH_3SO_3]	0.32396
49	1-ethyl-2,3-dimethyl imidazolium acetate	[EMM'Im][OAc]	0.32251
50	1-propyl-1-methyl piperidinium ethane sulfonate	[PMPip][$C_2H_5SO_3$]	0.32179
51	1-ethyl-1-methyl pyrrolidinium methyl sulfate	[EMPyrl][$MeSO_4$]	0.32009
51	1,1-dimethyl pyrrolidinium ethyl sulfate	[MM'Pyrl][$EtSO_4$]	0.32009
53	1-ethyl-2,3-dimethyl imidazolium propionate	[EMM'Im][C_2COO]	0.31828
54	1-butyl-1-methyl pyrrolidinium bisulfate	[BMPyrl][HSO_4]	0.31795
55	1-propyl-2,3-dimethyl imidazolium methane sulfonate	[PMM'Im][CH_3SO_3]	0.31637
56	1-butyl-2,3-dimethyl imidazolium acetate	[BEMM'Im][OAc]	0.31517
57	1-propyl-2,3-dimethyl imidazolium ethane sulfonate	[PMM'Im][$C_2H_5SO_3$]	0.31420
58	1,1-dimethyl pyrrolidinium bisulfate	[MM'Pyrl][HSO_4]	0.31253
59	1-ethyl-2,3-dimethylimidazolium butyrate	[EMM'Im][C_3COO]	0.31243
60	1-butyl-1-methyl piperidinium acetate	[BMPip][OAc]	0.31173
61	1-butyl-3-methyl imidazolium propionate	[BMIm][C_2COO]	0.31094
61	1-butyl-2,3-dimethyl imidazolium propionate	[BMM'Im][C_2COO]	0.31094
63	1-butyl-2,3-dimethyl imidazolium butyrate	[BMM'Im][C_3COO]	0.30509
64	1-butyl-3-methyl pyridinium bisulfate	[BMPyr][HSO_4]	0.30383
65	1,1-dimethyl pyrrolidinium methane sulfonate	[MM'Pyrl][CH_3SO_3]	0.30374
66	1-propyl-1-methyl pyrrolidinium bisulfate	[PMPyrl][HSO_4]	0.30222
67	1-propyl-1-methyl pyrrolidinium methyl sulfate	[PMPyrl][$MeSO_4$]	0.30202
68	1-propyl-3-methyl imidazolium bisulfate	[PMIm][HSO_4]	0.30049
68	1-methyl-3-propyl imidazolium bisulfate	[BPIm][HSO_4]	0.30049
70	1-butyl-4-methyl pyridinium bisulfate	[B4MPyr][HSO_4]	0.29943
71	1-butyl-3-methyl pyridinium acetate	[B3MPyr][OAc]	0.29772
72	1-butyl-1-methyl pyrrolidinium acetate	[BMPyrl][OAc]	0.29769
73	1-butyl-3-methyl pyridinium propionate	[B3MPyr][C_2COO]	0.29655
74	1-propyl-3-methyl pyridinium bisulfate	[PMPyr][HSO_4]	0.29604
74	1-methyl-3-propyl pyridinium bisulfate	[MPPyr][HSO_4]	0.29604
76	1-butyl-2-methyl pyridinium propionate	[B2MPyr][C_2COO]	0.29432
77	1-propyl-1-methyl pyrrolidinium methane sulfonate	[P<Pyrl][CH_3SO_3]	0.29344
78	1-propyl-1-methyl pyrrolidinium ethane sulfonate	[PMPyrl][$C_2H_5SO_3$]	0.29126
79	1-butyl imidazolium acetate	[BIm][OAc]	0.28952
80	1-butyl-2-methyl pyridinium butyrate	[B_2MPyr][C_3COO]	0.28846

81	1,2-diethyl pyridinium ethyl sulfate	[EE'Pyr][EtSO4]	0.28722
82	2-ethyl-1-methyl pyridinium methyl sulfate	[E'M'Pyr][$MeSO_4$]	0.28607
83	1-propyl-3-methyl imidazolium methyl sulfate	[PMIm][$MeSO_4$]	0.28590
84	1-ethyl pyridinium bisulfate	[Epyr][HSO_4]	0.27773
85	1-ethyl-3-methyl pyridinium bisulfate	[EMPyr][HSO_4]	0.27594
86	1-butyl pyridinium bisulfate	[BPyr][HSO_4]	0.27502
87	1-propyl imidazolium acetate	[PIm][OAc]	0.26912
88	Methyl propionate	[MeC_2COO]	0.25653
89	1-butyl-1-ethyl pyrrolidinium ethyl sulfate	[BEPyrl][$EtSO_4$]	0.24016
90	1-butyl-1-methyl pyrrolidinium methyl sulfate	[BMPyrl][$MeSO_4$]	0.23901
91	1-butyl-3-methyl imidazolium methyl sulfate	[BMIm][$MeSO_4$]	0.23619
92	1,1-Dimethyl piperidinium methyl sulfate	[MM'Pip][$MeSO_4$]	0.23503
92	1-ethyl-1-methyl piperidinium ethyl sulfate	[EMPip][$EtSO_4$]	0.23503
94	1-propyl-2,3-dimethyl imidazolium ethyl sulfate	[PMM'Im][$EtSO_4$]	0.23328
95	1-propyl-2,3-dimethyl imidazolium methyl sulfate	[PMM'Im][$MeSO_4$]	0.23213
96	1-butyl-1-methyl pyrrolidinium propionate	[BMPyrl][C_2COO]	0.22858
97	1-ethyl-3-methyl pyridinium methyl sulfate	[EMPyr][$MeSO_4$]	0.22407
97	1-butyl-3-methyl pyridinium methyl sulfate	[BMPyr][$MeSO_4$]	0.22407
99	1-butyl-1-methyl pyrrolidinium Butyrate	[BMPyrl][C_3COO]	0.22272
100	1,3-diethyl imidazolium methyl sulfate	[EE'Im][$MeSO_4$]	0.22251
101	1,3-dimethyl imidazolium methyl sulfate	[MM'Im][$MeSO_4$]	0.22197
102	1-propyl-3-methyl imidazolium acetate	[PMIm][OAc]	0.21535
103	1-butyl-4-methyl pyridinium acetate	[B4MPyr][OAc]	0.21429
104	1,3-dimethyl imidazolium acetate	[MM'Im][OAc]	0.21065
105	1-butyl-4-methyl pyridinium propionate	[B4MPyr][$EtSO_4$]	0.21006
106	1-butyl-4-methyl pyridinium methyl sulfate	[B4MPyr][$MeSO_4$]	0.20936
107	1-ethyl-3-methyl pyridinium ethyl sulfate	[EMPyr][EtSO4]	0.20873
108	1-butyl-3-methyl pyridinium butyrate	[B3MPyr][C_3COO]	0.20860
109	1,3-dimethyl pyridinium methyl sulfate	[MM'Pyr][$MeSO_4$]	0.20758
110	1-methyl-3-propyl pyridinium propionate	[MPPyr][C_2COO]	0.20667
111	1,3-dimethyl imidazolium propionate	[MM'Im][C_2COO]	0.20642
112	1-ethyl imidazolium acetate	[EIm][OAc]	0.20572
113	1-ethyl-1-methyl pyrrolidinium ethyl sulfate	[EMPyrl][$EtSO_4$]	0.20566
114	1-propyl-3-methyl imidazolium butyrate	[PMIm][C_3COO]	0.20526
115	1-methyl imidazolium acetate	[MIm][OAc]	0.20519
116	1,1-dimethyl pyrrolidinium methyl sulfate	[MM'Pyrl][$MeSO_4$]	0.20450
117	1-ethyl pyridinium ethyl sulfate	[Epyr][$EtSO_4$]	0.20445
118	1-butyl-4-methyl pyridinium butyrate	[B4MPyr][C_3COO]	0.20420
119	1,1,3,3-tetramethyl guanidinium acetate	[TMG][OAc]	0.20383
120	1-methyl pyridinium methyl sulfate	[MPyr][$MeSO_4$]	0.20330
121	1-butyl-2-methyl pyridinium acetate	[B2MPyr][OAc]	0.20262
122	1-methyl-3-propyl pyridinium butyrate	[MPPyr][C_3COO]	0.20081
123	1,3-dimethyl imidazolium butyrate	[MM'Im][C_3COO]	0.20057
124	1,1,3,3-tetramethyl guanidinium propionate	[TMG][C_2COO]	0.19960

125	1,1,3,3-tetramethyl guanidinium butyrate	[TMG][C_3COO]	0.19374
126	1-butyl pyridinium acetate	[Bpyr][OAc]	0.19258
127	1-ethyl-3-methyl pyridinium acetate	[EMPyr][OAc]	0.19079
128	1-ethyl pyridinium acetate	[Epyr][OAc]	0.18987
129	1-butyl pyridinium propionate	[Bpyr][C_2COO]	0.18836
130	1-methyl pyrrolidinium acetate	[MPyrl][OAc]	0.18771
131	1-ethyl-3-methyl pyridinium propionate	[EMPyr][C_2COO]	0.18657
132	Pyridinium acetate	[Pyr][OAc]	0.18652
133	1-ethyl pyridinium propionate	[Epyr][C_2COO]	0.18565
134	1-butyl-1-methyl pyrrolidinium methane sulfonate	[BMPyrl][CH_3SO_3]	0.18553
135	1-ethyl-3-methyl imidazolium butyrate	[EMIm][C_3COO]	0.18515
136	1-Methyl-2-pyrrolidinium propionate	[MPyrl][C_2COO]	0.18350
137	1-butyl-1-methyl pyrrolidinium ethane sulfonate	[BMPyrl][$C_2H_5SO_3$]	0.18336
138	1-butyl pyridinium butyrate	[Bpyr][C_3COO]	0.18250
139	Pyridinium propionate	[Pyr][C_2COO]	0.18229
140	1-ethyl-3-methyl pyridinium butyrate	[E3MPyr][C_3COO]	0.18071
141	1-ethyl pyridinium butyrate	[Epyr][C_3COO]	0.17979
142	1-butyl-3-methyl pyridinium methane sulfonate	[BMPyr][CH_3SO_3]	0.17141
143	1-butyl-3-methyl pyridinium ethane sulfonate	[BMPyr][$C_2H_5SO_3$]	0.16923
144	1-propyl-3-methyl imidazolium methane sulfonate	[PMIm][CH_3SO_3]	0.16808
145	1-butyl-4-methyl pyridinium methane sulfonate	[BM4Pyr][CH_3SO3]	0.16702
146	1-propyl-3-methyl imidazolium ethane sulfonate	[PMIm][$C_2H_5SO_3$]	0.16590
147	1-butyl-2,3-dimethyl imidazolium methane sulfonate	[BMM'Im][CH_3SO_3]	0.16574
148	1,1,3,3-tetramethyl guanidinium bisulfate	[TMG][HSO_4]	0.16534
149	1-butyl-4-methyl pyridinium ethane sulfonate	[B4MPyr][CH_3SO_3]	0.16484
150	1-propyl-3-methyl pyridinium methane sulfonate	[PMPyr][CH_3SO_3]	0.16362
150	1-methyl-3-propyl pyridinium methane sulfonate	[MPPyr][CH_3SO_3]	0.16362
152	1-butyl-2,3-dimethyl imidazolium ethane sulfonate	[BMM'Im][$C_2H_5SO_3$]	0.16356
153	2-hydroxyethyl ammonium propionate	2-HEAP	0.16236
154	1-ethyl-2,3-dimethyl imidazolium methane sulfonate	[EMM'Im][CH_3SO_3]	0.16210
155	1-propyl-3-methyl pyridinium ethane sulfonate	[PMPyr][$C_2H_5SO_3$]	0.16145
155	1-methyl-3-propyl pyridinium ethane sulfonate	[MPPyr][$C_2H_5SO_3$]	0.16145
157	1,3-dimethyl imidazolium ethane sulfonate	[MM'Im][$C_2H_5SO_3$]	0.16120
158	Formaldehyde	[HCHO]	0.15802
159	1,1,3,3-tetramethyl guanidinium methane sulfonate	[TMG][CH_3SO_3]	0.15656
160	1-butyl-2-methyl pyridinium methane sulfonate	[B2MPyr][CH_3SO_3]	0.15535
161	1,1,3,3-tetramethyl guanidinium ethane sulfonate	[TMG][C2H_5SO_3]	0.15438

162	1-butyl-2-methyl pyridinium ethane sulfonate	[B2MPyr][$C_2H_5SO_3$]	0.15318
163	1-butyl-3-methyl imidazolium butyrate	[BMIm][C_3COO]	0.15014
164	1-ethyl-3-methyl pyridinium methane sulfonate	[EMPyr][CH_3SO_3]	0.14352
165	1-butyl pyridinium ethane sulfonate	[BPyr][$C_2H_5SO_3$]	0.14313
166	1-ethyl pyridinium methane sulfonate	[Epyr][CH_3SO_3]	0.14261
167	1-ethyl-3-methyl pyridinium ethane sulfonate	[EMPyr][$C_2H_5SO_3$]	0.14135
168	1-ethyl pyridinium ethane sulfonate	[Epyr][$C_2H_5SO_3$]	0.14043
169	1-ethyl-3-methyl imidazolium ethyl sulfate	[EMIm][$EtSO_4$]	0.13865
170	1,3-diethyl imidazolium ethyl sulfate	[EE'Im][$EtSO_4$]	0.12095
171	1,3-dimethyl imidazolium methane sulfonate	[MM'Im][CH_3SO_3]	0.11622
172	1-ethyl-3-methyl imidazolium methyl sulfate	[EMIm][$MeSO_4$]	0.11466
173	1-ethyl-2,3-dimethyl imidazolium ethane sulfonate	[EMM'Im][$C_2H_5SO_3$]	0.11393
174	1-butyl-3-methyl imidazolium ethane sulfonate	[BMIm][$C_2H_5SO_3$]	0.11077
175	1-ethyl-3-methyl imidazolium methane sulfonate	[EMIm][CH_3SO_3]	0.10899
176	1-ethyl-3-methyl imidazolium bisulfate	[EMIm][HSO_4]	0.10828
177	1-ethyl-3-methyl imidazolium acetate	[EMIm][OAc]	0.10728
178	1-methyl imidazolium hydrogen sulfate	[MIm][HSO_4]	0.10711
179	1-butyl-3-methyl imidazolium methane sulfonate	[BMIm][CH_3SO_3]	0.10621
180	1,2,3-trimethyl imidazolium methyl sulfate	[MM'M''Im][$MeSO_4$]	0.10492
181	1-ethyl-3-methyl imidazolium ethane sulfonate	[EMIm][$C_2H_5SO_3$]	0.10270
182	Acetic acid	[CH_3COOH]	0.09746
183	butanol	[BuOH]	0.09710
184	1-butyl-3-methyl imidazolium acetate	[BMIm][OAc]	0.09453
185	1-butyl-3-methyl imidazolium bisulfate	[BMIm][HSO_4]	0.08245
186	1-ethyl-2,3-dimethyl imidazolium ethyl sulfate	[EMM'Im][$EtSO_4$]	0.08120
187	1-ethyl-3-methyl imidazolium propionate	[EMIm][C_2COO]	0.07818
188	1,3-dimethyl imidazolium ethyl sulfate	[MM'Im][$EtSO_4$]	0.07193
189	ethanolamine	[$EtNH_2$]	0.06912

Supplementary Materials: The following are available online at www.mdpi.com/xxx/s1, Table S1: Table lists the HF-ILs that were studied for analysis in this work and their corresponding raw materials, Table S2: Criteria, parameters describing the ionic liquids along with their weighting factors, Table S3: Table showing the results of TOPSIS analysis for raw materials, comparison with traditional organic solvents and ionic liquids combined with sensitivity analysis for changes in range of ±10%. For the sake of brevity, the relative closeness to the ideal solution, ranking, ranking difference for ± 10% sensitivity changes are represented separately. Table S4: Overall ranking of the halide free ILs

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