

The Electrical Conductivity of Ionic Liquids: Machine Learning Approaches

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Supplementary Material File S1

Database information

Table S1 presents all details for data origin and characteristics, created with data from NIST IL-Thermo database [1,2]. Details on experimental methods incorporated can be found in the respective references. The database is also provided in *xls* file, as Supplementary Material No.2.

Table S1. The database of ILs incorporated for our model, with 2274 data points

Name	Chemical formula	Experimental method	Data points	Ref.
1-butyl-1-methylpyrrolidinium dicyanamide	$C_{11}H_{20}N_4$	Alternating current cell with electrodes	140	[3]
1-ethyl-3-methylimidazolium tetrafluoroborate	$C_6H_{11}BF_4N_2$	Alternating current cell with electrodes	183	[4]
triethyl (pentyl) phosphonium bis((trifluoromethyl) sulfonyl) amide	$C_{13}H_{26}F_6NO_4PS_2$	Electrochemical impedance spectroscopy	79	[5]
1-butyl-3-methylimidazolium tetrafluoroborate	$C_8H_{15}BF_4N_2$	EC cell	74	[6]
1-butyl-1-methylpyrrolidinium bis[(trifluoromethyl) sulfonyl]imide	$C_{11}H_{20}F_6N_2O_4S_2$	Direct current cell with electrodes	56	[7]
1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl) imide	$C_{10}H_{15}F_6N_3O_4S_2$	Direct current cell with electrodes	56	[7]
1-methyl-3-octylimidazolium tetrafluoroborate	$C_{12}H_{23}BF_4N_2$	Alternating current cell with electrodes	54	[8]
1-octyl-3-methylimidazolium hexafluorophosphate	$C_{12}H_{23}F_6N_2P$	Alternating current cell with electrodes	54	[8]
1-butyl-3-methylimidazolium hexafluorophosphate	$C_8H_{15}F_6N_2P$	Syringe-type cell	51	[9]
ethylammonium nitrate	$C_2H_8N_2O_3$	Alternating current cell with electrodes	44	[10]
1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	$C_{10}H_{15}F_6N_3O_4S_2$	Alternating current cell with electrodes	51	[11]
1-ethyl-3-methylimidazolium bromide	$C_6H_{11}BrN_2$	Alternating current cell with electrodes	44	[4]
1-hexadecyl-3-methylimidazolium tetrafluoroborate	$C_{20}H_{39}BF_4N_2$	Alternating current cell with electrodes	40	[4]
1-ethyl-3-methylimidazolium 4-methylbenzenesulfonate	$C_{13}H_{18}N_2O_3S$	Alternating current cell with electrodes	40	[4]
triethyl(pentyl)phosphonium bis((trifluoromethyl)sulfonyl)amide	$C_{13}H_{26}F_6NO_4PS_2$	electrochemical impedance spectroscopy	38	[5]
1-ethyl-3-methylimidazolium tetrafluoroborate	$C_6H_{11}BF_4N_2$	Alternating current cell with electrodes	36	[12]
1-ethyl-3-methylimidazolium ethyl sulfate	$C_8H_{16}N_2O_4S$	Alternating current cell with electrodes	36	[12]
triethylhexylammonium bis((trifluoromethyl)sulfonyl)imide	$C_{14}H_{28}F_6N_2O_4S_2$	Crison GLP31	34	[13]
1-methyl-2-oxopyrrolidin-1-ium sulfurochloridate	$C_5H_{10}ClNO_4S$	Alternating current cell with electrodes	33	[14]
1-decyl-3-methylimidazolium tetrafluoroborate	$C_{14}H_{27}BF_4N_2$	Alternating current cell with electrodes	33	[4]
1-methyl-1-propylpyrrolidinium bis[(trifluoromethyl)sulfonyl]imide	$C_{10}H_{18}F_6N_2O_4S_2$	Alternating current cell with electrodes	32	[15]

1-butyl-1-methylpyrrolidinium bis((trifluoromethyl)sulfonyl)imide	C ₁₁ H ₂₀ F ₆ N ₂ O ₄ S ₂	Alternating current cell with electrodes	32	[15]
1-methyl-1-octylpyrrolidinium bis(trifluoromethylsulfonyl)amide	C ₁₅ H ₂₈ F ₆ N ₂ O ₄ S ₂	Alternating current cell with electrodes	32	[15]
1-ethyl-3-methylimidazolium hexafluorophosphate	C ₆ H ₁₁ F ₆ N ₂ P	Alternating current cell with electrodes	32	[4]
1-hexyl-1-methylpyrrolidinium bis(trifluoromethanesulfonyl)imide	C ₁₃ H ₂₄ F ₆ N ₂ O ₄ S ₂	Alternating current cell with electrodes	29	[15]
1-butyl-3-methylimidazolium bis(perfluoroethylsulfonyl)imide	C ₁₂ H ₁₅ F ₁₀ N ₃ O ₄ S ₂	Alternating current cell with electrodes	29	[16]
1-butyl-3-methylimidazolium bis(fluorosulfonyl)imide	C ₈ H ₁₅ F ₂ N ₃ O ₄ S ₂	Alternating current cell with electrodes	29	[16]
1-methyl-3-octylimidazolium bis(trifluoromethylsulfonyl)imide	C ₁₄ H ₂₃ F ₆ N ₃ O ₄ S ₂	Alternating current cell with electrodes	29	[16]
1-ethyl-3-methylimidazolium chloride	C ₆ H ₁₁ ClN ₂	Alternating current cell with electrodes	29	[4]
1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	C ₁₀ H ₁₅ F ₆ N ₃ O ₄ S ₂	Alternating current cell with electrodes	28	[7]
1-methyl-3-octylimidazolium tetrafluoroborate	C ₁₂ H ₂₃ BF ₄ N ₂	Alternating current cell with electrodes	27	[9]
3-octyl-1H-imidazol-3-ium bis((trifluoromethyl)sulfonyl)amide	C ₁₃ H ₂₁ F ₆ N ₃ O ₄ S ₂	Alternating current cell with electrodes	25	[17]
3-decyl-1H-imidazol-3-ium bis((trifluoromethyl)sulfonyl)amide	C ₁₅ H ₂₅ F ₆ N ₃ O ₄ S ₂	Alternating current cell with electrodes	25	[17]
3-butyl-1H-imidazol-3-ium bis((trifluoromethyl)sulfonyl)amide	C ₉ H ₁₃ F ₆ N ₃ O ₄ S ₂	Alternating current cell with electrodes	25	[17]
3-dodecyl-1H-imidazol-3-ium bis((trifluoromethyl)sulfonyl)amide	C ₁₇ H ₂₉ F ₆ N ₃ O ₄ S ₂	Alternating current cell with electrodes	25	[17]
3-hexyl-1H-imidazol-3-ium bis((trifluoromethyl)sulfonyl)amide	C ₁₁ H ₁₇ F ₆ N ₃ O ₄ S ₂	Alternating current cell with electrodes	25	[17]
N-octyl-3-methylpyridinium tetrafluoroborate	C ₁₄ H ₂₄ BF ₄ N	Conductimeter from CRISON, model GLP31	25	[18]
1-butyl-4-methylpyridinium tetrafluoroborate	C ₁₀ H ₁₆ BF ₄ N	Conductimeter from CRISON, model GLP31	25	[18]
1-butylpyridinium tetrafluoroborate	C ₉ H ₁₄ BF ₄ N	Conductimeter from CRISON, model GLP31	25	[18]
1-butyl-3-methylpyridinium tetrafluoroborate	C ₁₀ H ₁₆ BF ₄ N	Conductimeter from CRISON, model GLP31	25	[18]
1-propylpyridinium tetrafluoroborate	C ₈ H ₁₂ BF ₄ N	Conductimeter from CRISON, model GLP31	25	[19]
2-methyl-1-propylpyridinium bis((trifluoromethyl)sulfonyl)amide	C ₁₁ H ₁₄ F ₆ N ₂ O ₄ S ₂	Conductimeter from CRISON, model GLP31	25	[20]

1-ethyl-2-methylpyridinium bis((trifluoromethyl)sulfonyl)amide	$C_{10}H_{12}F_6N_2O_4S_2$	Conductimeter from CRISON, model GLP31	25	[20]
1-octyl-3-methylimidazolium hexafluorophosphate	$C_{12}H_{23}F_6N_2P$	Alternating current cell with electrodes	25	[9]
1-methyl-1-propylpyrrolidinium bis(fluorosulfonyl)amide	$C_8H_{18}F_2N_2O_4S_2$	Alternating current cell with electrodes	25	[21]
1-ethyl-3-methyl-1H-imidazolium bis(fluorosulfonyl)amide	$C_6H_{11}F_2N_3O_4S_2$	Alternating current cell with electrodes	25	[21]
1-ethyl-3-methylimidazolium octyl sulfate	$C_{14}H_{28}N_2O_4S$	Alternating current cell with electrodes	24	[22]
1-methyl-3-octylimidazolium tetrafluoroborate	$C_{12}H_{23}BF_4N_2$	Alternating current cell with electrodes	24	[23]
1-butyl-3-methylimidazolium tetrafluoroborate	$C_8H_{15}BF_4N_2$	Alternating current cell with electrodes	24	[23]
1-hexyl-3-methylimidazolium tetrafluoroborate	$C_{10}H_{19}BF_4N_2$	Alternating current cell with electrodes	24	[23]
1-ethyl-3-methylimidazolium tetrafluoroborate	$C_6H_{11}BF_4N_2$	Alternating current cell with electrodes	23	[23]
1-dodecyl-3-methylimidazolium tetrafluoroborate	$C_{16}H_{31}BF_4N_2$	Alternating current cell with electrodes	23	[4]
1-butyl-3-methylimidazolium dicyanamide	$C_{10}H_{15}N_5$	Alternating current cell with electrodes	23	[24]
triethylsulfonium bis((trifluoromethyl)sulfonyl)imide	$C_8H_{15}F_6NO_4S_3$	Alternating current cell with electrodes	22	[25]
1-butyl-3-methylpyridinium dicyanamide	$C_{12}H_{16}N_4$	Conductimeter from CRISON, model GLP31	21	[18]
1-butyl-2-methylpyridinium tetrafluoroborate	$C_{10}H_{16}BF_4N$	Conductimeter from CRISON, model GLP31	21	[18]
1-ethylpyridinium bis[(trifluoromethyl)sulfonyl]imide	$C_9H_{10}F_6N_2O_4S_2$	Conductimeter from CRISON, model GLP31	21	[26]
N-methyl-N-propylpyrrolidinium acetate	$C_{10}H_{21}NO_2$	Alternating current cell with electrodes	21	[27]
N-methyl-N-propylpyrrolidinium lactate	$C_{11}H_{23}NO_3$	Alternating current cell with electrodes	21	[27]
1-butyl-1-methylpyrrolidinium dicyanamide	$C_{11}H_{20}N_4$	Alternating current cell with electrodes	21	[25]
1-butyl-3-methylimidazolium trifluoromethanesulfonate	$C_9H_{15}F_3N_2O_3S$	Alternating current cell with electrodes	21	[24]
1-butyl-3-methylimidazolium hexafluorophosphate	$C_8H_{15}F_6N_2P$	Alternating current cell with electrodes	21	[24]
1-hexyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	$C_{12}H_{19}F_6N_3O_4S_2$	Alternating current cell with electrodes	20	[16]
1-ethyl-3-methylimidazolium tris(pentafluoroethyl)trifluorophosphate	$C_{12}H_{11}F_{18}N_2P$	Alternating current cell with electrodes	20	[16]

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