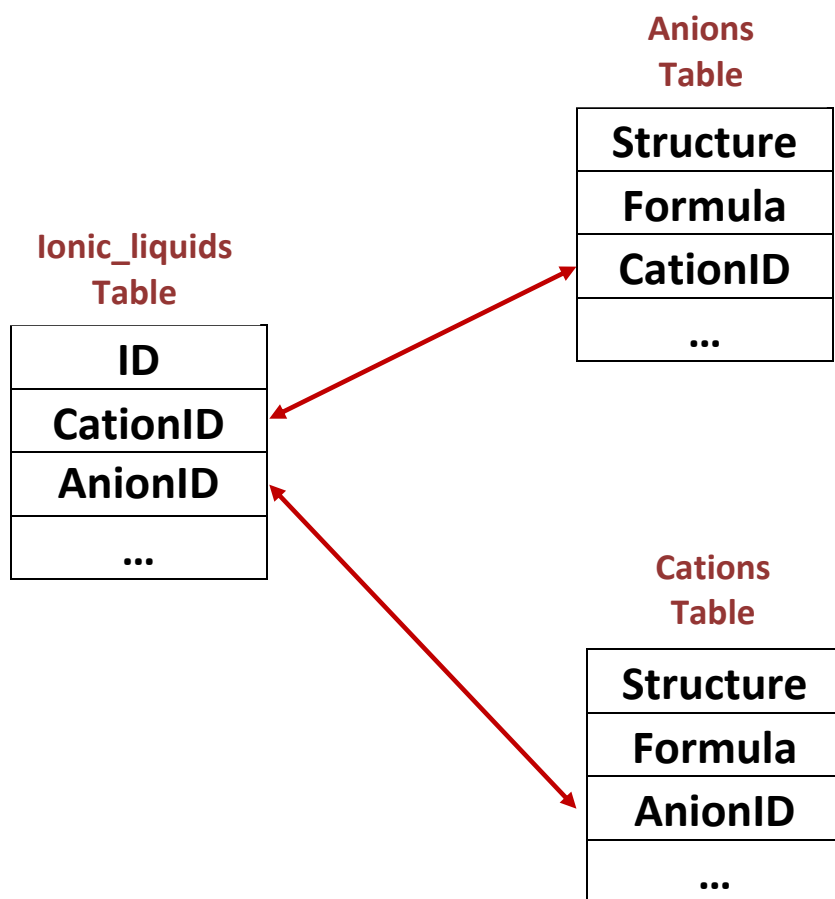


IJC Exercise: Database for Ionic liquids

C. Muller, G. Marcou, A. Varnek

Create a new project with InstantJChem representing the proposed tables and relationships (foreign keys). At the end, generate a view where all table are shown.

General Schema.

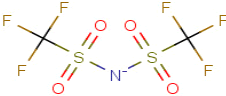
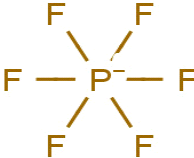
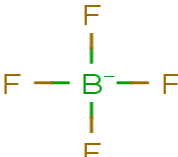


Red arrows represent relationships between tables.

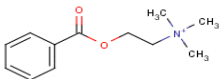
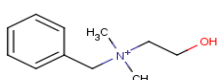
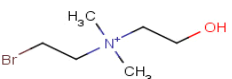
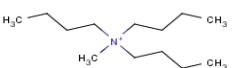
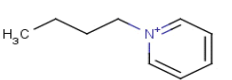
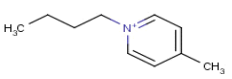
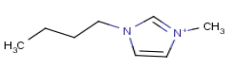
- Ionic_liquids Table

ID	CationID	AnionID	cation	anion	Viscosity	T_Viscosity	date
1	1	1	Bz-COOC ₂ H ₄ N(CH ₃) ₃	Tf ₂ N	6570,00	25	01/01/2007
2	2	1	Me ₂ NBz(C ₂ H ₄ OH)	Tf ₂ N	762,00	25	01/01/2007
3	3	1	Me ₂ N(C ₂ H ₄ Br)(C ₂ H ₄ OH)	Tf ₂ N	626,00	25	01/01/2007
7	6	2	N-butyl-4 picolinium	PF ₆	140,00	45	01/01/2007
202	6	3	4-methyl-N butyl pyridinium	BF ₄	80,85	40	01/01/2007
369	5	3	1-butylpyridinium	BF ₄			01/01/2007
370	5	1	1-butylpyridinium	Tf ₂ N			01/01/2007
465	4	2	(butyl)3methylN	PF ₆			01/01/2007
824	8	1	C ₄ -mim	Tf ₂ N			05/01/2009
825	8	3	C ₄ -mim	BF ₄	75,00	30	05/01/2009
827	8	2	C ₄ -mim	PF ₆	182,00	30	05/01/2009

- Anions Table

Structure	Mol Weight	Formula	AnionID	ShortName	LongName
	280,15	C ₂ F ₆ NO ₄ S ₂	1	Tf ₂ N	bis(trifluoromethylsulfonyl)azanide
	144,96	F ₆ P	2	PF ₆	hexafluorophosphate
	86,81	BF ₄	3	BF ₄	tetrafluoroborate

- Cations Table

Structure	Mol Weight	Formula	CationID	ShortName	LongName
	208,28	C ₁₂ H ₁₈ NO ₂	1	Bz-COOC ₂ H ₄ N(CH ₃) ₃	2-benzoyloxyethyl(trimethyl)ammonium
	180,27	C ₁₁ H ₁₈ NO	2	Me ₂ NBz(C ₂ H ₄ OH)	benzyl(2-hydroxyethyl)dimethylammonium
	197,09	C ₆ H ₁₅ BrNO	3	Me ₂ N(C ₂ H ₄ Br)(C ₂ H ₄ OH)	(2-bromoethyl)(2-hydroxyethyl)dimethylammonium
	200,38	C ₁₃ H ₃₀ N	4	MeBu ₃ N	(1-methyl)(1,1,1-tributyl)ammonium
	136,21	C ₉ H ₁₄ N	5	N-butyl pyridinium	1-butyl-pyridin-1-ium
	150,24	C ₁₀ H ₁₆ N	6	N-butyl-4 picolinium	1-butyl-4-methylpyridin-1-ium
	139,22	C ₈ H ₁₅ N ₂	8	Bumim	1-butyl-3-methyl-1H-imidazol-3-ium