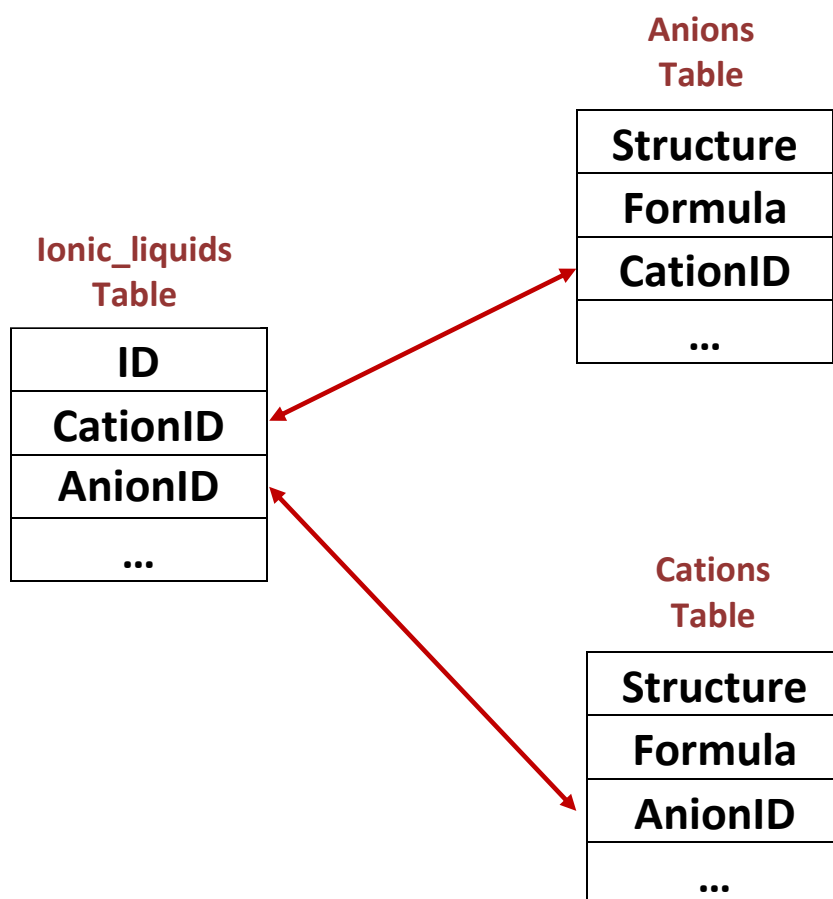


IJC Exercise: Database for Ionic liquids

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.

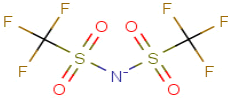
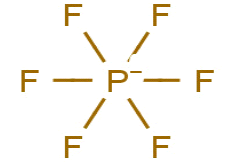
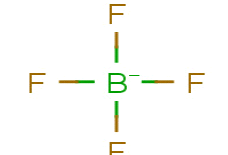


Red arrows represent relationships between tables.

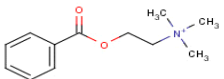
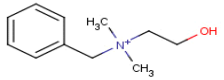
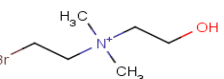
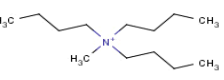
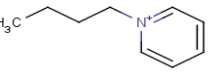
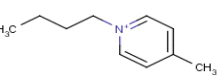
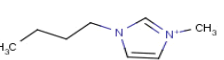
- Ionic_liquids Table

| ID | CationID | AnionID | cation | anion | Viscosity | T_Viscosity | date |
|-----|----------|---------|-----------------------------|-------|-----------|-------------|------------|
| 1 | 1 | 1 | Bz-COOC2H4N(CH3)3 | Tf2N | 6570,00 | 25 | 01/01/2007 |
| 2 | 2 | 1 | Me2NBz(C2H4OH) | Tf2N | 762,00 | 25 | 01/01/2007 |
| 3 | 3 | 1 | Me2N(C2H4Br)(C2H4OH) | Tf2N | 626,00 | 25 | 01/01/2007 |
| 7 | 6 | 2 | N-butyl-4 picolinium | PF6 | 140,00 | 45 | 01/01/2007 |
| 202 | 6 | 3 | 4-methyl-N butyl pyridinium | BF4 | 80,85 | 40 | 01/01/2007 |
| 369 | 5 | 3 | 1-butylpyridinium | BF4 | | | 01/01/2007 |
| 370 | 5 | 1 | 1-butylpyridinium | Tf2N | | | 01/01/2007 |
| 465 | 4 | 2 | (butyl)3methylN | PF6 | | | 01/01/2007 |
| 824 | 8 | 1 | C4-mim | Tf2N | | | 05/01/2009 |
| 825 | 8 | 3 | C4-mim | BF4 | 75,00 | 30 | 05/01/2009 |
| 827 | 8 | 2 | C4-mim | PF6 | 182,00 | 30 | 05/01/2009 |

- Anions Table

| Structure | Mol Weight | Formula | AnionID | ShortName | LongName |
|---|------------|-----------|---------|-----------|-------------------------------------|
|  | 280,15 | C2F6NO4S2 | 1 | Tf2N | bis(trifluoromethylsulfonyl)azanide |
|  | 144,96 | F6P | 2 | PF6 | hexafluorophosphate |
|  | 86,81 | BF4 | 3 | BF4 | 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 |