

```

{
  "reactants" : {
    "O" : {} ,
    "NO2" : {}
  },
  "products" : {
    "NO" : {}
  },
  "type" : "ARRHENIUS",
  "A" : 5.6E-12,
  "B" : 0.0E+00,
  "C" : 180.0
}

```

(a) Arrhenius reaction

```

{
  "name" : "n-butanol",
  "type" : "CHEM_SPEC",
  "UNIFAC groups" : {
    "OH" : 1,
    "CH2(-OH)" : 1,
    "CH2(hydrophobic tail)" : 2,
    "CH3(hydrophobic tail)" : 1
  }
  ...
},
{
  "name" : "n-butanol/water activity",
  "type" : "SUB_MODEL_UNIFAC",
  "phases" : [ "n-butanol/water mixture" ],
  "functional groups" : {
    "CH2(-OH)" : {
      "main group" : "CHn(-OH)",
      "volume param" : 0.6744,
      "surface param" : 0.540
    },
    "CH2(hydrophobic tail)" : {
      "main group" : "CHn(hydrophobic tail)",
      "volume param" : 0.6744,
      "surface param" : 0.540
    },
    ...
  },
  "main groups" : {
    "CHn(-OH)" : {
      "interactions with" : {
        "OH" : 986.5,
        "H2O" : 2314
      }
    },
    "OH" : {
      "interactions with" : {
        "CHn(-OH)" : 156.4,
        "CHn(hydrophobic tail)" : 156.4,
        "H2O" : 276.4
      }
    },
    ...
  }
}

```

(b) UNIFAC activity model