# MD Simulation Data supporting the publication “Hydrogen Bond Redistribution Effects in Mixtures of Protic Ionic Liquids Sharing the Same Cation: Nonideal Mixing With Large Negative Mixing Enthalpies”

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## 1. General Information:

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| Dataset title | MD Simulation Data supporting the publication “Hydrogen Bond Redistribution Effects in Mixtures of Protic Ionic Liquids Sharing the Same Cation: Nonideal Mixing With Large Negative Mixing Enthalpies” |
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## 2. Description:

The following data set belongs to the publication [1]. It includes the force field and parameter files as well as start configurations which were used to run molecular dynamics simulations with Gromacs 5.0.6. of the mixture of [TEA][OTf] with [TEA][OMs]. Furthermore, the calculated excess enthalpies as well as densities, potential energies and fractions of hydrogen bonds between the TEA-cation and the OTf-anion or OMs-anion are given. For more information, check the README.txt file.

## 3. Archive Structure:

There is a README.txt with further information, as well as two directories: **results** and **setup**.
In **results**, you can find all the molecular dynamics simulation information from the SI of the publication [1]. You find 11 .csv files named xoms_x.x.csv, where x.x is replaced with the mole

fraction of [TEA][OMs], e.g. xoms_0.1.csv for a mole fraction of x(OMs) = 0.1. As a function of temperature, the following calculated properties are listed: density, potential energy, fraction of hydrogen bonds between the cation and OMs-anions/OTf-anions. Furthermore, you find the file **excess_energies_of_mixing.csv**. Here the excess energies of mixing as well as the errors are documented in two tables. For more details on how the properties were calculated, please check the publication [1]. All files are .csv files and readable with a simple editor.

In **setup** all information about the set-up of the simulations are documented. This includes .mdp-parameter files for the equilibration, as well as the production runs, the force fields files and configuration files. The simulations were done with Gromacs 5.0.6. For naming conventions, please check the Gromacs user manual [2]. All files are readable with a simple editor.

## 4. References:

[1] “Hydrogen Bond Redistribution Effects in Mixtures of Protic Ionic Liquids Sharing the Same Cation: Nonideal Mixing with Large Negative Mixing Enthalpies”, *Benjamin Golub, Daniel Ondo, Viviane Overbeck, Ralf Ludwig, Dietmar Paschek,* Physical Chemistry Chemical Physics, 2022, **DOI: 10.1039/D2CP01209J**

[2]M. J. Abraham, D. van der Spoel, E. Lindahl, B. Hess, and the GROMACS development team. GROMACS User Manual version 5.0.6, 2015.