Molecular Modelling of a Mechanochemical reaction: The Case of 18-Crown-6 Ether and KCl

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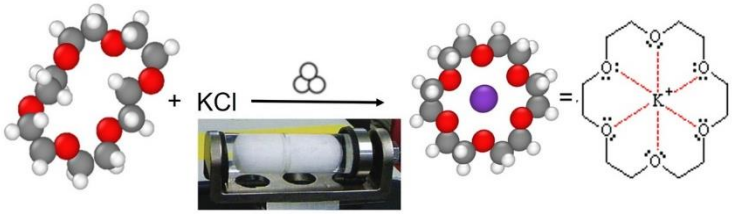
Mechanochemistry is the area of chemistry that deals with transformations induced and/or aided by mechanical force [1]. The most common method employed in modern mechanochemistry is through ball milling (BM) but the inherent nature of it makes it difficult to experimentally investigate individual impacts due to moving parts and provide a molecular-level insight [2]. Therefore, molecular dynamics (MD) simulations come into play to provide a better picture.



Using Gromacs 2021.5 package, MD simulations were performed to understand milling mechanisms, analyse the deformations on crystal and evolution of a ball milling reaction. Two neutral, non-reactive and rigidly constrained balls were incorporated into our simulating model to induce mechanical force via inelastic collisions The solid-state mechanochemical complexation reaction between 18c6 and potassium chloride (KCl) was used as a model for our simulations. This integrated approach, wherein MD simulations helps in visualizing, validating experimental results and providing molecular level insight, contributes to a more holistic understanding of mechanochemical reactions.

[1] James, S.L. et al. Mechanochemistry: opportunities for new and cleaner synthesis. Chem. Soc. Rev. 41, 413–447 (2012).
[2] Carta, M., Vugrin, L., Miletić, G., Kulcsár, M. J., Ricci, P. C., Halasz, I., & Delogu, F. (2023). Mechanochemical reactions from individual impacts to global transformation kinetics. *Angewandte Chemie International Edition*, 62(33), e202308046.