DECODING MECHANOHEMICAL DRIVERS

Experimental Isolation of Single Impact, Cumulative Energy, Aging and Liquid-Assisted Grinding Effect*

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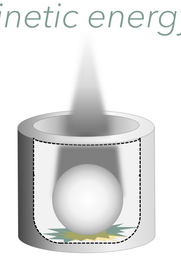
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Single Impact Energy (E_{impact})

kinetic energy

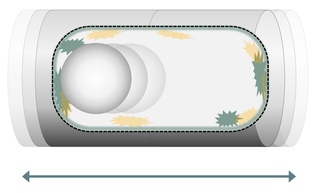


parameter dependency

frequency | time | ball weight

Cumulative Energy (E_{total})

kinetic energy over time

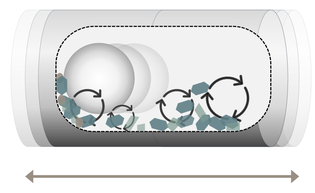


parameter dependency

frequency | time | ball weight

Physical Mixing

particle translocation

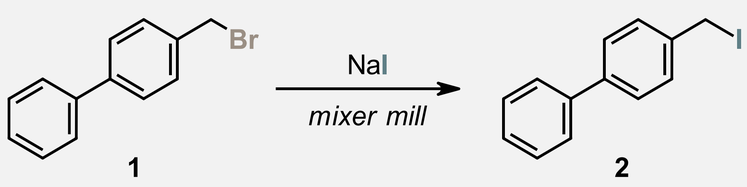


parameter dependency

frequency | time | ball weight

Systematic variation of ball milling parameters **frequency | time | ball weight** identified the driving factors for mechanochemical reactions.

The Finkelstein Reaction



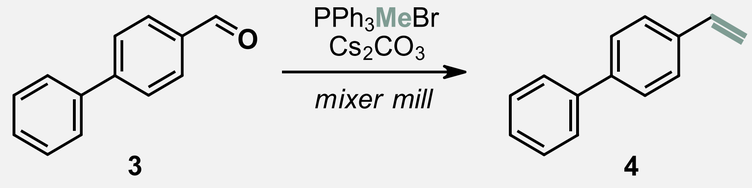
Experimental Setup

All-solid reactants, solvent-free conditions.

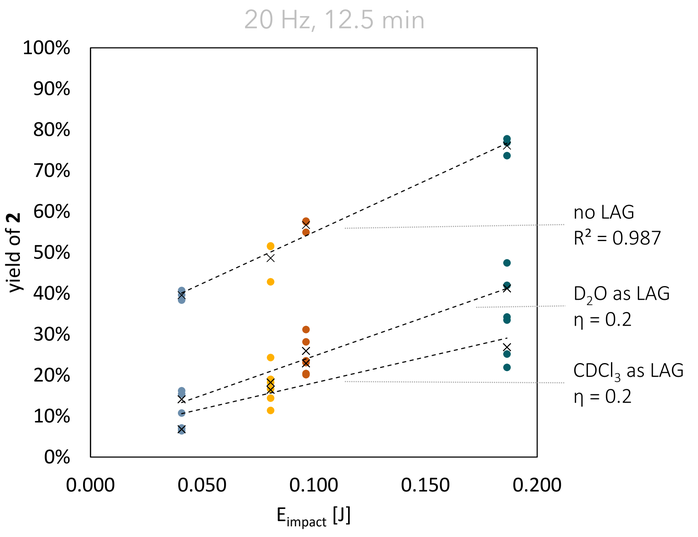
NO LIQUID MICROENVIRONMENTS!

Chemical conversion is triggered by milling.

The Wittig Olefination



Are Mechanochemical Reactions Driven by the Single Impact Energy (E_{impact}) or Physical Mixing?

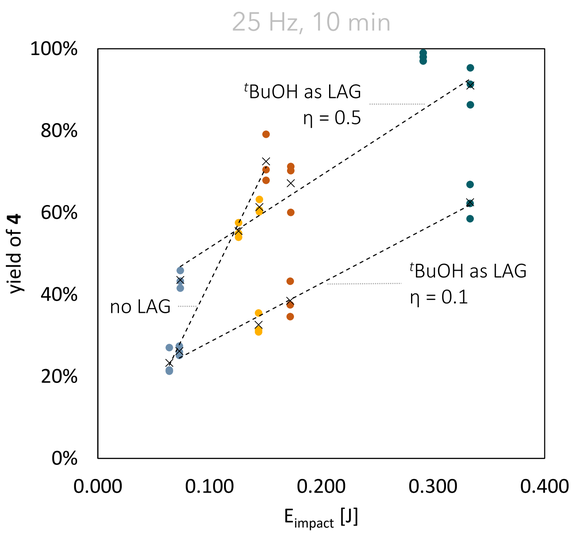


frequency | time | **ball weight**

as varied parameter

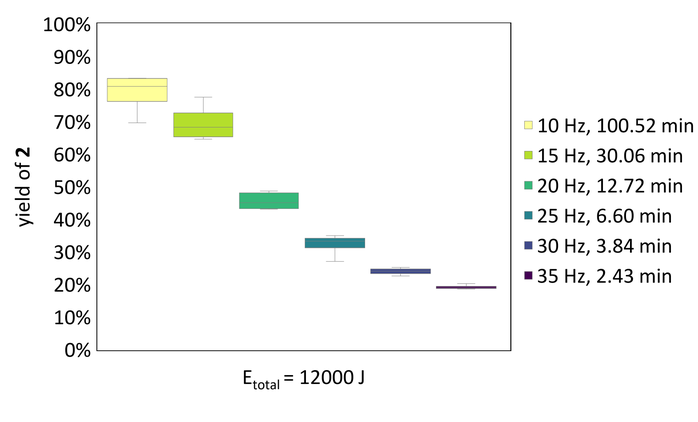
15 mm Milling Ball	Material Density [g/cm³]	Ball Mass [g]	E_{impact} [J]
Silicon Nitride	3.20	5.742	0.064
Zirconia	6.10	11.348	0.126
Chrome Steel	7.70	13.576	0.151
Tungsten Carbide	14.90	26.239	0.291

constant parameters: number of milling balls | ball/jar dimension | filling degree



Mechanochemical reactions are **impact-driven** and physical mixing does not primarily govern the reaction.
Enhanced diffusion by **liquid-assisted grinding (LAG)** does not substitute for the impact-driven regime

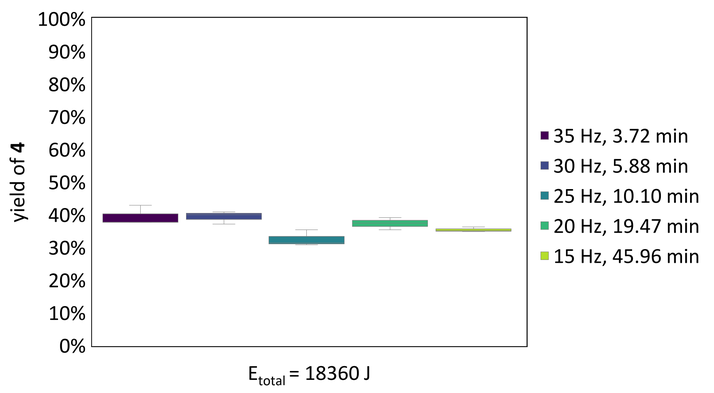
Is the Cumulative Energy (E_{total}) a Valid Parameter to Predict the Yield of Mechanochemical Reactions?

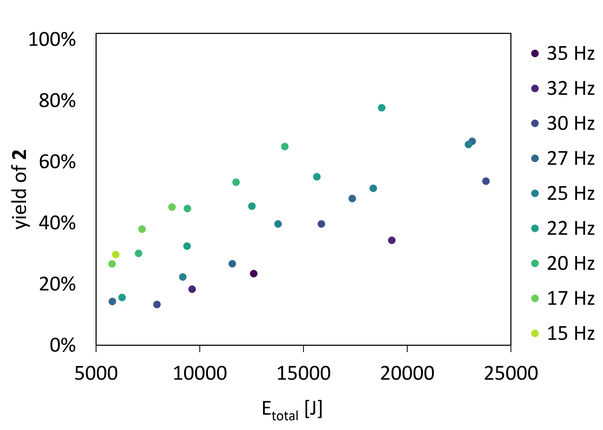


frequency | time | ball weight

as varied parameter

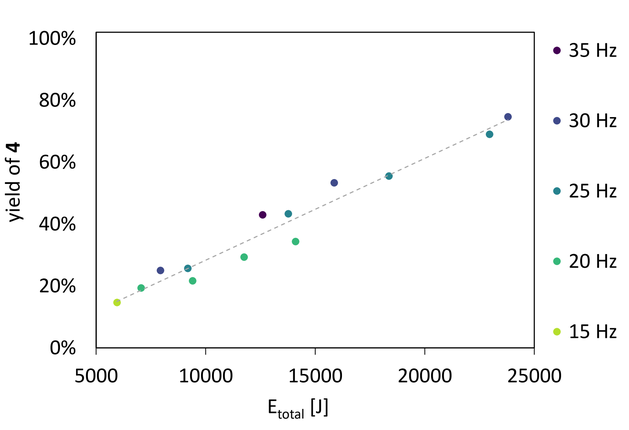
In the **Finkelstein Reaction (left)** the yield does **NOT** scale with E_{total} as the reaction ages.





In the **Wittig Olefination (right)** the yield scales **LINEARLY** with E_{total}.

AGING. The chemical transformation continues after mechanical activation.



The mechanochemical yield scales **linearly** with the cumulative Energy ($\mathbf{E_{total}}$) if non-linear effects are absent.

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