

Nanographenes by Solvent-free Syntheses - The Mechanochemical Scholl Reaction

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Nanographenes and graphene nanoribbons are promising materials with potential applications in organic and nano-electronics.[1] During the bottom-up synthesis of these nanographenes the Scholl reaction [2,3], a Lewis-acid catalysed oxidative cyclodehydrogenation is utilized to planarize precursor systems by forming aryl-aryl bonds and creating a fully pi-conjugated material. Especially for the larger precursors solubility is a main concern but even the smallest planarized hexabenzocoronene (HBC) is basically insoluble in common organic solvents. The common workaround is the introduction of solubilizing groups, resulting in additional synthesis steps. Thereby, the atom economy of the process suffers, hindering the scale-up needed for industrial applications.

This contribution is illuminating a radical new approach towards the planarization of nanographenes utilizing a mechanochemical Scholl reaction. Our approach is displaying a tremendous advance in terms of both ecological and economic aspects, since the mechanochemical synthesis requires neither hazardous solvents nor harsh reaction conditions and can be conducted within a short time scale.[4,5] Moreover, our synthetic pathway excels in scalability and versatility significantly broadening the synthetic prospects towards larger extended nanographenes.

The mechanochemically Scholl reaction is elucidated by conducting a detailed study of the milling process. In addition, an in-situ study of pressure and temperature during the milling process was conducted. Furthermore, the versatility of our approach is demonstrated by expanding it to two

other benchmark nanographenes triangular shaped C₆₀ and C₂₂₂. This new reaction route paves the way towards larger extended nanographenes and graphene nanoribbons and renders the introduction of solubilizing groups obsolete.

References

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Figures

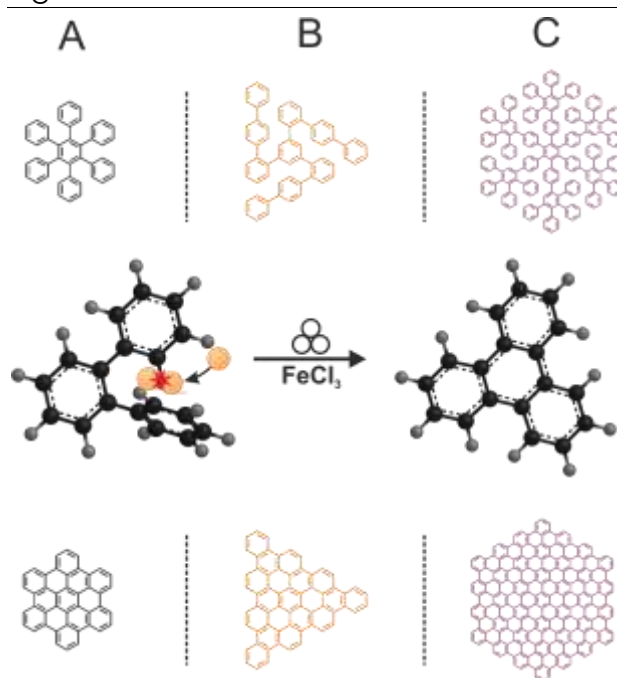


Figure 1: Scholl reaction of different precursors (C₄₂H₂₆ (A); C₆₀H₄₂ (B); C₂₂₂H₁₅₀ (C)) with iron(III) chloride in a planetary ball mill to produce the benchmark PAHs HBC, triangular-shaped C₆₀ and C₂₂₂.