

Benzene Coupling and Solvent-free Birch-type Reduction Driven by a Mechanochemically Synthesised Electride

Nathan Davison¹, James Quirk¹, Floriana Tuna², David Collison², Claire L. McMullin^{3*}, Hannes Michaels^{1,4}, Harvey Morrill⁵, Paul G. Waddell¹, Jamie A. Gould¹, Marina Freitag¹, James A. Dawson^{1*}, Erli Lu^{1*}

Affiliations:

¹ Chemistry–School of Natural and Environmental Sciences, Newcastle University, Newcastle upon Tyne, UK, NE1 7RU.

² Department of Chemistry, The University of Manchester, Oxford Road, UK, Manchester M13 9PL.

³ Department of Chemistry, University of Bath, Claverton Down, Bath, UK, BA2 7AY.

⁴ Department of Chemistry – Ångström Laboratory, Uppsala University, Uppsala 75120, Sweden.

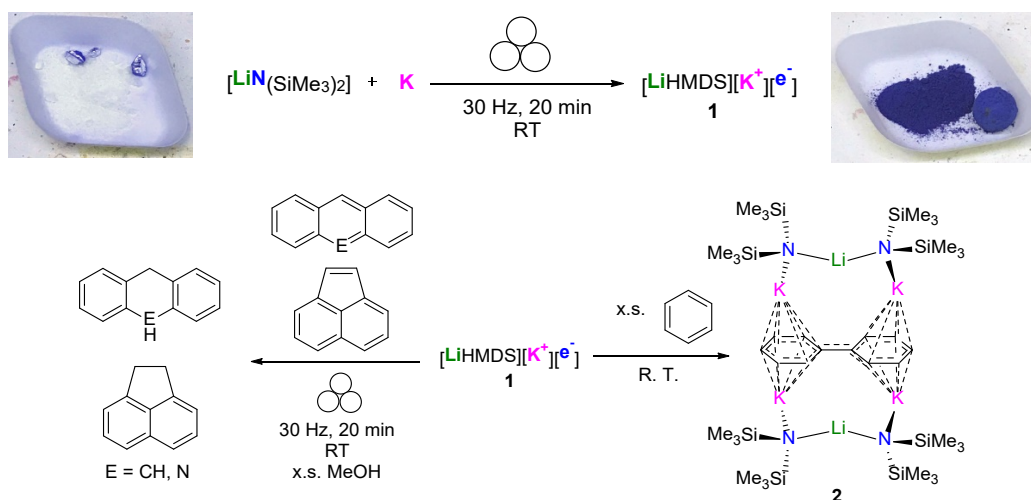
⁵ School of Mathematics, Statistics and Physics, Newcastle University, Newcastle upon Tyne, UK, NE1 7RU.

e-mail: n.davison1@newcastle.ac.uk

Abstract

Delivering challenging chemical transformations under mild conditions with non-hazardous low-cost reagents/catalysts is arguably one of the strongest motivations of chemistry research. Benzene coupling into biphenyl and arene/heteroarene Birch-type reduction are two important classes of reaction. However, these require either transition metal catalysts or harsh or hazardous conditions.¹⁻³

Using mechanochemistry, a group 1 metal electride (a type of compound featuring free electrons as the anion),⁴ was synthesised. The electride, [LiHMDS][K⁺][e⁻] (**1**), was found to have an unprecedented three-dimensional helical electron topology.⁵ This electride delivers challenging reactions at mild and sustainable conditions, such as benzene coupling to form a biphenyl dianion complex (**2**) and the first solvent-free Birch reductions at room temperature.



References

- [1] A. J. Birch, *J. Chem. Soc.*, 1944, 430-436.
- [2] J. A. Ashenurst, *Chem. Soc. Rev.*, 2010, **39**, 540-548.
- [3] C. S. Yeung and V. M. Dong, *Chem. Rev.*, 2011, **111**, 1215-1292.
- [4] J. L. Dye, *Acc. Chem. Res.*, 2009, **42**, 1564-1572.
- [5] C. Liu, S. A. Nikolaev, W. Ren and L. A. Burton, *J. Mater. Chem. C*, 2020, **8**, 10551-10567.