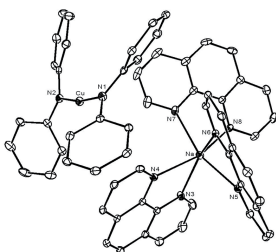


can work as an effective catalyst to carry out the C-N coupling under the same reaction conditions indicating that **2** is the intermediate of the catalytic system. Both  $[\text{Cu}(\text{NPh}_2)_2]^-$  and  $[\text{Cu}(\text{NPh}_2)\text{I}]^-$  were observed by *in situ* electrospray ionization mass spectrometry (ESI-MS) analysis under the catalytic reaction condition indicating that they are intermediates in the reaction. A catalytic cycle was proposed based on these observations. Molecular structure of **2** was determined by single-crystal X-ray diffraction analysis.



**Keywords:** C-N coupling, copper, ESI-MS

## MS52.P01

*Acta Cryst.* (2011) **A67**, C557

### Effect of thermal treatment on characteristics nanodiamonds and diamond blend

Svetlana N. Ivashevskaya,<sup>a</sup> Vasily A. Lebedev,<sup>b</sup> Gennady P. Kopitsa,<sup>c</sup> <sup>a</sup>*Institute of Geology Karelian Research Centre RAS, Petrozavodsk (Russia).* <sup>b</sup>*Department of Materials Science, Moscow State University, Moscow (Russia).* <sup>c</sup>*Petersburg Nuclear Physics Institute RAS, 188300 Gatchina (Russia).* E-mail: ivashevskaja@yahoo.com

Diamond nanoparticles are now the most commonly synthesized nanomaterials. As they have some distinctive properties, such as high adsorptive capacity, high thermal conductivity, high surface energy, hydrophobicity and a large specific surface, they are of great interest as materials with a wide application range. Nanodiamonds (NDs) can be used as adsorbents and catalysts for the production of nanocomposite materials, for growing diamond films, in medicine and biotechnology [1-3]. They can not now be widely used mainly because there are no well-defined standards and the quality of the NDs, offered by different producers, is unstable [4]. Therefore, the study of NDs is important and promising.

The main goal of NDs purification is removal of non-diamond forms of carbon. Practically all known methods are based on the use of the different resistances of diamond and non-diamond forms of carbon to oxidants. To apply them, many technical problems, arising in exothermal reactions at high temperatures and intensive gassing in a limited volume, should be solved [5]. A decisive factor in selecting a purification variant is safety.

The goal of the project was to assess the effect of thermal treatment in vacuum on the structural characteristics and chemical composition of NDs and a diamond blend produced by detonation synthesis. NDs in the form of powders were obtained from two sources: Gansu Liru Lingyun NanoMaterial Co Ltd. (China) and NanoCarbon Research Institute Ltd. (Japan). A diamond blend (brand AIII-A) was offered by Scientific and Technical Enterprise "Sinta" (Belarus).

It is commonly accepted that only a complex of diagnostic techniques gives the possibility to get a true knowledge about the carbon nanostructures properties. Chemical composition was determined by mass-spectrometry (an inductively-coupled plasma mass-spectrometer ICP-MS Xseries2 (ThermoFisher Scientific)) and X-ray spectral analysis (a VEGA II LSH electron microscope (TESCAN OJSC) with an attachment for microprobe analysis); different levels of structural elements aggregation were analysed by SEM (VEGA II LSH), AFM (N'Tegra Aura NT-MDT) and DLS (Malvern Instruments Ltd.) methods; structural parameters of crystallites were analysed by X-ray structural analysis (Thermo Scientific ARL X'TRA Powder X-ray Diffraction System); in order to determine the pair density-density

correlation functions and to estimate parameters of the nanostructure (correlation length, specific surface and fractal dimension) was used SANS.

Our study has shown that thermal treatment under mild conditions is a promising approach to purification of NDs and a diamond blend from the point of view of economy, safety and environmental protection.

*The project was supported by ESD RAS-5.*

[1] O. Shenderova, V.V. Zhirnov, D.W. Brenner, *Crit. Rev. Solid State Mater.* **2002**, *27*, 227 [2] A.M. Schrand, H. Huang, C. Carlson, J.J.Schlager, *Phys. Chem. B.* **2007**, *111*, 2. [3] V.J. Dolmatov, L.N. Kostrova, *Superhard materials* **2000**, *3*, 82. [4] V. Teslenko <http://rough-polished.com/ru/analytics/31816.html> **2009**. [5] V.G. Sushchev, V.J. Dolmatov, V.A. Marchukov, M.V.Veretennikova [www.rql.kiev.ua/almaz\\_j](http://www.rql.kiev.ua/almaz_j), **2008**.

**Keywords:** carbon, nanotechnology, diamond

## MS52.P02

*Acta Cryst.* (2011) **A67**, C557-C558

### Synthesis of nanographene organometallics for deposition on a graphene surface

Andrew Parlett,<sup>a</sup> Paul Raithby,<sup>a</sup> Adelina Ilie,<sup>b</sup> Gavin Jones,<sup>b</sup> Sara Fuentes,<sup>a</sup> Simon Bending,<sup>b</sup> <sup>a</sup>*Department of Chemistry,* <sup>b</sup>*Department of Physics, University of Bath (UK).* Email: ap292@bath.ac.uk

Graphene's unique electrical and mechanical properties give it a wide variety of possible applications in the future of electronic devices [1]. Being essentially an extended network of interconnected arene rings, it is also of much interest in chemistry. It can be modified chemically via oxidation, (partial) hydrogenation etc to alter the band gap, or else used as a surface on which to adsorb small molecules which can be visualised using AFM and STM microscopy. Such small molecule adsorption can be used for reactions directed by the graphene surface or for functionalising the graphene [2].

We have successfully synthesised a range of organometallic compounds with coordinated polycyclic aromatic hydrocarbons (or nanographenes) such as pyrene which are either novel or found as a new polymorph. These compounds have been characterised using a variety of spectroscopic methods, as well as X-ray crystallography. These compounds will be deposited on to graphite or graphene and imaged using AFM and STM microscopy. This will allow us to optimise the surface coverage of such molecules and analyse their interactions with the surface and each other. By 'sticking' molecules such as these to graphene we hope to be able to alter the electrical, magnetic and optical properties of graphene.

