

Dataset for ‘Understanding the AC conductivity and permittivity of trapdoor chabazites for future development of next-generation gas sensors’: Information

Hélène Bordeneuve^{a,1}, Dominic J. Wales^{b,1,2}, Andrew J.W. Physick^b, Huan V. Doan^{c,d}, Valeska P. Ting^c and Chris R. Bowen^{a,3}

^a Department of Mechanical Engineering, University of Bath, Claverton Down, Bath, Somerset, BA2 7AY, United Kingdom

^b Department of Chemical Engineering, University of Bath, Claverton Down, Bath, Somerset, BA2 7AY, United Kingdom

^cDepartment of Mechanical Engineering, University of Bristol, Bristol, BS8 1TR, United Kingdom

^dDepartment of Oil Refining and Petrochemistry, Faculty of Oil and Gas, Hanoi University of Mining and Geology, Duc Thang, Bac Tu Liem, Hanoi, Viet Nam

This dataset contains raw data from the study published as ‘Understanding the AC conductivity and permittivity of trapdoor chabazites for future development of next-generation gas sensors’ in *Microporous Mesoporous Mater.*, (2018), **260**, 208-216.

Thermogravimetric analysis (TGA) data: The raw thermogravimetric analysis (TGA) data for synthetic K⁺ chabazite (KCHA), Cs⁺ chabazite (CsCHA) and Zn²⁺ chabazite (ZnCHA) is included in Excel spreadsheet files. The TGA data were collected on a Setaram Setsys Evolution on sample masses of ~5 mg. The samples were submitted to heating and cooling cycles from room temperature (~21 °C) to 700 °C at a 5 °C min⁻¹ heating rate under a flow of air. For all the TGA data Excel spreadsheet files the data for each parameter and chabazite sample is clearly labelled in the different worksheets and in the columns within the worksheets.

Electrochemical data: The AC conductivity data, permittivity and phase angle data (given as Excel spreadsheet files) for the three different chabazite materials was calculated from the raw complex impedance data, using formulae given by Bowen, Buschhorn and Adamaki (Bowen *et al.* 2014). The raw complex impedance data was collected using was measured in the frequency range 0.1 Hz – 1 MHz using a Solartron 1260 Impedance analyzer with a 1296 Dielectric Interface, over a range of temperatures from room temperature (~21 °C) to 710 °C. A two phase heating profile was used to ensure dehydration of the samples, *i.e.* the samples were first heated to 710 °C whilst complex impedance data was collected and then the samples were allowed to cool back to room temperature (~21 °C) also whilst complex impedance data was collected. The AC conductivity during the cooling phase was used to enable calculation of the cation migration activation energies. For all the electrochemical data Excel spreadsheet files the data for each parameter and chabazite sample is clearly labelled in the different worksheets and in the columns within the worksheets.

¹ Joint first authorship

² Present Address: Faculty of Engineering, University of Nottingham, University Park Campus, Nottingham, NG7 2RD, United Kingdom. Email: dominic.wales@nottingham.ac.uk

³ Corresponding author: E-mail address: c.r.bowen@bath.ac.uk (C.R. Bowen).

Powder X-ray diffractometry (XRD) data: Powder X-ray diffractometry, for identification and phase purity determination, was performed using a Phillips SEI diffractometer with a CuK α source ($\lambda = 1.540598 \text{ \AA}$). For all the powder X-ray diffractometry data Excel spreadsheet files the data for each parameter and chabazite sample is clearly labelled in the different worksheets and in the columns within the worksheets.

Reference:

Bowen, C.R., Buschhorn, S. & Adamaki, V., 2014. Manufacture and characterization of conductor-insulator composites based on carbon nanotubes and thermally reduced graphene oxide. *Pure Appl. Chem.*, 86(5), pp.765–774.