**Direct Solid State NMR Observation of the 105Pd Nucleus in Inorganic Compounds and Palladium Metal Systems**

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This document serves as instructions for the location of the data within the directory **Hooper\_PCCP** **c8cp02594k \_105Pd data** available from the University of Warwick open access research data repository, WRAP (Warwick Research Archive Portal). This data directory contains the raw data files for all the data presented in the *Physical Chemistry Chemical Physics* manuscript entitled “Direct Solid State NMR Observation of the 105Pd Nucleus in Inorganic Compounds and Palladium Metal Systems“, (manuscript no. c8cp02594k).

The directory is seperated into subdirectories with names following the format below:

**Hooper\_PCCP\_data\FigX&Y\_[type]**

where FigX&Y denotes that the actual data utliised in Figures X and Y, and [type] provides further information about the type of data that it represents.

Each subdirectory is then separated into folders denoting the material system that the data was investigating with folders named with the following shorthand convention for each sample:

e.g. **K2PdBr6** = K2PdBr6(s), **PVPstabPd** = PVP stabilised Pd nanoparticles, etc.

All MAS and static NMR data (**Fig1&2&SI1&SI2\_105PdNMR\_complexes**; **Fig3\_39KNMR**; **Fig4\_35ClNMR**; **Fig6&SI3\_105PdNMR\_metals**)is initially categorised by seperating into folders representing the magnetic field strength at which the data was acquired (i.e. either **7.05T**, **9.40T**, **11.7T**, **14.1T** or **20.0T**). These MAS and static NMR data are predominantly in the form of raw Bruker TopSpin data folders with some **7.05T** data saved as text files (due to aquisition on a Varian-Chemagnetics spectrometer controlled by SPINSIGHT software). For the 105Pd VOCS NMR measurements the raw data of each individual spectrum that contributes to the cumulative/total spectrum has been included. The spectrometer frequency of each spectrum has been appended to the end of the VOCS file names in brackets (i.e. **170125\_300(26.63MHz)**) to differentiate between them. (N.B. the file names of NMR data begin with the date followed by an arbitrary number X such as **YYMMDD\_X**).

The PDF data (**Fig5\_PDF**) is given as a text file and the produced structure is included as a CIF file, while the TEM images (**Fig7\_TEM**) are given as JPG or PNG files.