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| **File Name** | **File Type** |  | **Description** |
| ex situ catalyst characterisation | Microsoft Excel Worksheet | Sheet 1 - XRD | X-ray Diffraction patterns of catalyst samples Pd/γ-Al2O3-ex(NO3) and Pd/γ-Al2O3-ex(NH3) |
|  |  |  | Sherrer Calculation of crystallite size |
|  |  |  | Database XRD patterns of reference files: 00-002-1420, 00-001-1201 and 00-002-1432 |
|  |  | Sheet 2 - Raman | Normalised Raman Emission spectra of catalyst samples Pd/γ-Al2O3-ex(NO3) and Pd/γ-Al2O3-ex(NH3) |
|  |  |  | Raw data emission spectra of 6 different positions from each sample |
|  |  |  | Integration report for peak area between 690 cm-1 and 600 cm-1 |
|  |  | Sheet 3 - Catalytic activity | CH4 concentration collected from FTIR detector during methane oxidation test and corresponding CH4 %conversion |
|  |  | Sheet 4 - FTIR CO Adsorption | Background subtracted FTIR absorption values of catalyst samples Pd/γ-Al2O3-ex(NO3) and Pd/γ-Al2O3-ex(NH3) after pulsing with carbon monoxide |
| exsitu EXAFS\_Calcined Catalysts | Microsoft Excel Worksheet | Sheet 1 - norm( E) | Normalised XAFS spectra of catalyst Pd/γ-Al2O3-ex(NO3), Pd/γ-Al2O3-ex(NH3), Pd foil ference and PdO reference sample at room temperature |
|  |  | Sheet 2 - normderivE | Derivativative (normalised XAFS spectra/X-ray energy) of catalyst Pd/γ-Al2O3-ex(NO3), Pd/γ-Al2O3-ex(NH3), Pd foil ference and PdO reference sample at room temperature |
|  |  | Sheet 3 - k2 chi | k2 weighted EXAFS spectra of catalyst Pd/γ-Al2O3-ex(NO3), Pd/γ-Al2O3-ex(NH3), Pd foil ference and PdO reference sample at room temperature |
|  |  | Sheet 4 - R plots | Fourier transformed EXAFS spectra of catalyst Pd/γ-Al2O3-ex(NO3), Pd/γ-Al2O3-ex(NH3), Pd foil ference and PdO reference sample at room temperature |
|  |  | Sheet 5 - Fitting parameter | Parameters for coordination number (CN), coordination distance ( R) and EXAFS Debye Waller factor (ss) of fits to the EXAFS data of Pd/γ-Al2O3-ex(NO3) and Pd/γ-Al2O3-ex(NH3) using scattering paths Pd-O, Pd-Pd1 and Pd-Pd2 of PdO |
|  |  | Sheet 6 - Fitting Plots | Magnitude and imaginary components of a fit to Pd/γ-Al2O3-ex(NO3) and Pd/γ-Al2O3-ex(NH3) using scattering paths Pd-O, Pd-Pd1 and Pd-Pd2 of PdO |
| exsitu EXAFS\_Reduced catalysts H2 | Microsoft Excel Worksheet | Sheet 1 - R plots | Fourier transformed EXAFS spectra of catalyst Pd/γ-Al2O3-ex(NO3), Pd/γ-Al2O3-ex(NH3) and Pd foil after reduction treatment in H2 atmosphere |
|  |  | Sheet 2 - Fitting Parameters | Parameters for coordination number (CN), coordination distance ( R) and EXAFS Debye Waller factor (ss) of fits to the EXAFS data of reduced Pd/γ-Al2O3-ex(NO3) and Pd/γ-Al2O3-ex(NH3) in H2 atmosphere using a single scattering path Pd-Pd of Pd metal |
|  |  | Sheet 3 - Particle Size caluclation | Calculation of average Pd particle size using coordination numbers from the EXAFS fit |
|  |  | Sheet 4 - norm u(E ) | Normalised XAFS spectra of catalyst Pd/γ-Al2O3-ex(NO3), Pd/γ-Al2O3-ex(NH3) and Pd foil after reduction treatment in H2 atmosphere |
| in situ data | Microsoft Excel Worksheet | Sheet 1 - TGA | Thermogravimetric Analysis of of precursor samples Pd(NO3)2/γ-Al2O3 and Pd(NH3)4(OH)2/γ-Al2O3 under flowing air |
|  |  | Sheet 2 - MS | Mass spectrometry signal of effluent flow from Pd(NO3)2/γ-Al2O3 and Pd(NH3)4(OH)2/γ-Al2O3 during calcination ramp conditions |
| TEM\_Particle Size Analysis | Microsoft Excel Worksheet | Sheet 1 - PdAl2O3\_exNO3 | Diameter of 100 measured particles of catalyst sample Pd/γ-Al2O3-ex(NO3), and frequency count of particle size |
|  |  | Sheet 1 - PdAl2O3\_exNH3 | Diameter of 100 measured particles of catalyst sample Pd/γ-Al2O3-ex(NH3), and frequency count of particle size |
| MC7C\_Frame6 | TIF file |  | Transmission electron microscopy image of catalyst Pd/γ-Al2O3-ex(NO3) |
| MC120B\_Frame16 | TIF file |  | Transmission electron microscopy image of catalyst Pd/γ-Al2O3-ex(NH3) |
| Pd(NO3)2-Al2O3 DRIFTS | Microsoft Excel Worksheet | Sheet 1 - Ramp | Diffuse reflectance infrared absorption spectra of precursor Pd(NO3)2/γ-Al2O3 at increasing temperatures during ramping stage of calciantion treatment |
|  |  | Sheet 2 - Dwell | Diffuse reflectance infrared absorption spectra of precursor Pd(NO3)2/γ-Al2O3 during dwell period (500°C) of calcination treatment |
|  |  | Sheet 3 - Cool | Diffuse reflectance infrared absorption spectra of precursor Pd(NO3)2/γ-Al2O3 at decreasing temperatures during cooling stage of calciantion treatment |
| Pd(NH3)4(OH)2-Al2O3 DRIFTS | Microsoft Excel Worksheet | Sheet 1 - Ramp | Diffuse reflectance infrared absorption spectra of precursor Pd(NH3)4(OH)2/γ-Al2O3 at increasing temperatures during ramping stage of calciantion treatment |
|  |  | Sheet 2 - Dwell | Diffuse reflectance infrared absorption spectra of precursor Pd(NH3)4(OH)2/γ-Al2O3 during dwell period (500°C) of calcination treatment |
|  |  | Sheet 3 - Cool | Diffuse reflectance infrared absorption spectra of precursor Pd(NH3)4(OH)2/γ-Al2O3 at decreasing temperatures during cooling stage of calciantion treatment |
| EXAFS Pd(NO3)2-Al2O3 ramp | Microsoft Excel Worksheet | Sheet 1 | Fourier transformed EXAFS spectra of catalyst Pd/γ-Al2O3-ex(NO3) from XAFS data collected at increasing temperature during ramping stage of calcination treatment |
| EXAFS Pd(NO3)2-Al2O3 Initial | Microsoft Excel Worksheet | Sheet 1 - k2 chi | k2 weighted EXAFS spectra of precursor sample Pd(NO3)2/γ-Al2O3 and Pd(NO3)2 reference sample collected at room temperature |
|  |  | Sheet 2 - FT R plots | Fourier transformed EXAFS spectra of precursor sample Pd(NO3)2/γ-Al2O3 and Pd(NO3)2 reference sample collected at room temperature, Magnitude and imaginary components of a fit to Pd(NO3)2/Al2O3 using scattering paths Pd-O and Pd-Pd |
| EXAFS Pd(NO3)2-Al2O3 ramp | Microsoft Excel Worksheet | Sheet 1 - norm( E) | Normalised XAFS spectra of catalyst Pd/γ-Al2O3-ex(NO3) from XAFS data collected at decreasing temperature during cooling stage of calcination treatment |
|  |  | Sheet 2 - k2 chi | k2 weighted EXAFS spectra of catalyst Pd/γ-Al2O3-ex(NO3) from XAFS data collected at decreasing temperature during cooling stage of calcination treatment |
|  |  | Sheet 3 - R plots | Fourier transformed EXAFS spectra of catalyst Pd/γ-Al2O3-ex(NO3) from XAFS data collected at decreasing temperature during cooling stage of calcination treatment |
|  |  | Sheet 4 - change in ss with temp | Guessed EXAFS Debye Waller values (σ2) of the scattering paths Pd(O), Pd(Pd1) and Pd(Pd2) used in the fit of Pd/γ-Al2O3-ex(NO3) to PdO at decreasing temperatures |
| EXAFS Pd(NO3)2\_ramp\_203C | Artemis fitting project |  | EXAFS fit of Pd(NO3)2/γ-Al2O3 data collected at 203C during the calcination ramping treatment to fitting model using scattering paths of Pd-O and Pd-Pd |
| EXAFS Pd(NO3)2\_ramp\_213C | Artemis fitting project |  | EXAFS fit of Pd(NO3)2/γ-Al2O3 data collected at 213C during the calcination ramping treatment to fitting model using scattering paths of Pd-O and Pd-Pd |
| EXAFS Pd(NO3)2\_ramp\_223C | Artemis fitting project |  | EXAFS fit of Pd(NO3)2/γ-Al2O3 data collected at 223C during the calcination ramping treatment to fitting model using scattering paths of Pd-O and Pd-Pd |
| EXAFS Pd(NO3)2\_ramp\_233C | Artemis fitting project |  | EXAFS fit of Pd(NO3)2/γ-Al2O3 data collected at 233C during the calcination ramping treatment to fitting model using scattering paths of Pd-O and Pd-Pd |
| EXAFS Pd(NO3)2\_ramp\_243C | Artemis fitting project |  | EXAFS fit of Pd(NO3)2/γ-Al2O3 data collected at 243C during the calcination ramping treatment to fitting model using scattering paths of Pd-O and Pd-Pd |
| EXAFS Pd(NO3)2\_ramp\_253C | Artemis fitting project |  | EXAFS fit of Pd(NO3)2/γ-Al2O3 data collected at 253C during the calcination ramping treatment to fitting model using scattering paths of Pd-O and Pd-Pd |
| EXAFS Pd(NH3)4-Al2O3 Initial | Microsoft Excel Worksheet | Sheet 1 - k2 chi | k2 weighted EXAFS spectra of precursor sample Pd(NH3)4(OH)2/γ-Al2O3 and Pd(NH3)4(OH)2 reference sample collected at room temperature |
|  |  | Sheet 2 - FT R plots | Fourier transformed EXAFS spectra of precursor sample Pd(NH3)4(OH)2/γ-Al2O3 and Pd(NH3)4(OH)2 reference sample collected at room temperature, Magnitude and imaginary components of a fit to Pd(NH3)4(OH)2/γ-Al2O3 using single scattering path Pd-N |
| EXAFS Pd(NH3)4-Al2O3 ramp | Microsoft Excel Worksheet | Sheet 1 | Fourier transformed EXAFS spectra of catalyst Pd(NH3)4(OH)2/γ-Al2O3 from XAFS data collected at increasing temperature during ramping stage of calcination treatment |
| EXAFS Pd(NH3)(OH)2\_ramp\_403C | Artemis fitting project |  | EXAFS fit of Pd(NH3)4(OH)2/γ-Al2O3 data collected at 403C during the calcination ramping treatment to fitting model using scattering paths of Pd-O and Pd-Pd |
| EXAFS Pd(NH3)(OH)2\_ramp\_413C | Artemis fitting project |  | EXAFS fit of Pd(NH3)4(OH)2/γ-Al2O3 data collected at 413C during the calcination ramping treatment to fitting model using scattering paths of Pd-O and Pd-Pd |
| EXAFS Pd(NH3)(OH)2\_ramp\_423C | Artemis fitting project |  | EXAFS fit of Pd(NH3)4(OH)2/γ-Al2O3 data collected at 423C during the calcination ramping treatment to fitting model using scattering paths of Pd-O and Pd-Pd |
| EXAFS Pd(NH3)(OH)2\_ramp\_433C | Artemis fitting project |  | EXAFS fit of Pd(NH3)4(OH)2/γ-Al2O3 data collected at 433C during the calcination ramping treatment to fitting model using scattering paths of Pd-O and Pd-Pd |
| EXAFS Pd(NH3)(OH)2\_ramp\_443C | Artemis fitting project |  | EXAFS fit of Pd(NH3)4(OH)2/γ-Al2O3 data collected at 443C during the calcination ramping treatment to fitting model using scattering paths of Pd-O and Pd-Pd |
| EXAFS Pd(NH3)(OH)2\_ramp\_453C | Artemis fitting project |  | EXAFS fit of Pd(NH3)4(OH)2/γ-Al2O3 data collected at 453C during the calcination ramping treatment to fitting model using scattering paths of Pd-O and Pd-Pd |
| EXAFS Pd(NH3)(OH)2\_ramp\_463C | Artemis fitting project |  | EXAFS fit of Pd(NH3)4(OH)2/γ-Al2O3 data collected at 463C during the calcination ramping treatment to fitting model using scattering paths of Pd-O and Pd-Pd |