1. Introduction:
Selective hydrogenation of mixtures of 1,3-dienes obtained from the C2 cracking fraction of a petrochemical complex could be one method of obtaining high-value stereo-specific mono-olefins. This study examines whether catalysts displaying distinct stereoselective hydrogenation characteristics (isomerisation/hydrogenation) can be used to affect diene hydrogenation profiles.

2. Catalyst characterisation:
   - Catalyst prepared by the wet impregnation technique.
   - Characterised using pulsed CO chemisorption followed by CO temperature programmed desorption (TPD) using Hiden mass spectrometer (HPR-20 Q/C).
   - Calculated metal dispersion ~ 13.4% (Pd:CO = 2:1).
   - Low temperature CO peak (Tmax, 580 K) assigned to metal bond to Pd crystallites.
   - High temperature peak (Tmax, 650 K) assigned to decay of carboxy species associated with alumina support [1].

3. Experimental:
A modified Gaseby-Specac 5661 heated infrared gas cell housed within a Nicolet Avatar FTIR spectrometer was employed as a batch reactor. Purified helium and hydrogen flows were regulated by dedicated mass flow controllers. The catalyst was mounted on a glass boat and loaded into the reactor as described in Figure 1. The glass boat is located out of the beam path such that only gaseous components are analysed as the reaction proceeds.

5. Results:
Reaction profiles were constructed by examining the intensity of infrared bands uniquely diagnostic of each species present in the gas phase. A list of the diagnostic bands used to identify gaseous species is presented in the table below:

<table>
<thead>
<tr>
<th>Compound</th>
<th>Band position (cm⁻¹)</th>
<th>Width (cm⁻¹)</th>
<th>Assignment</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,3-pentadiene</td>
<td>689</td>
<td>w</td>
<td>aliphatic rock and CO-O deformation</td>
</tr>
<tr>
<td>trans-2-pentene</td>
<td>689</td>
<td>s</td>
<td>im, phase antisymmetric CH₃ stretch</td>
</tr>
<tr>
<td>cis-2-pentene</td>
<td>689</td>
<td>m</td>
<td>im, phase antisymmetric CH₃ stretch</td>
</tr>
<tr>
<td>1,5-pentadiene</td>
<td>1510</td>
<td>m</td>
<td>out-of-plane C=C stretch</td>
</tr>
<tr>
<td>trans-2-pentene</td>
<td>2916</td>
<td>w</td>
<td>im, phase antisymmetric CH₃ stretch</td>
</tr>
<tr>
<td>cis-2-pentene</td>
<td>2916</td>
<td>w</td>
<td>im, phase antisymmetric CH₃ stretch</td>
</tr>
</tbody>
</table>

5.1 Mono-olefins
Hydrogenation of trans-2-pentene:
Here, trans-2-pentene is directly converted to pentane (Figure 4). Analysis of the mass balance showed 69% of the incident moles of trans-2-pentene had been converted to pentane, with 31% of the hydrocarbon retained at the catalyst surface.

5.2 Di-olefins
Hydrogenation of cis-1,3-pentadiene:
Here, firstly, the terminal double bond is hydrogenated to produce trans-pent-2-ene. The internal bond is subsequently hydrogenated to produce pentane. No cis-pent-2-ene is detected. However, on completion of reaction, inspection of the mass balance shows 56% retention of the hydrocarbon at the catalyst surface. It is possible that any cis-pent-2-ene that might form in the initial step is selectively retained by the catalyst.

6. Conclusions:
Previous studies have shown first and second stage hydrogenation of 1,3-pentadiene on Pd/Al₂O₃ occurs at two distinct sites [3]. Work is currently underway to examine whether selective poisoning strategies can be used to block stage 2 hydrogenation, which would allow trans-1,3-pentadiene to be selectively hydrogenated to trans-pent-2-ene.