



## Characterisation of the SOFC material, $\text{LaCrO}_3$ , using vibrational spectroscopy

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### Abstract

$\text{LaCrO}_3$  is reported to undergo a low to high temperature (HT) phase transition from orthorhombic ( $Pnma$ ) to rhombohedral ( $R-3c$ ), at ca. 255 °C. The phases involved in the low temperature phase transition of  $\text{LaCrO}_3$  have been determined using Raman spectroscopy at temperatures from –196 to 300 °C. There are nine Raman bands observed from a total of 24 predicted modes, seven of which are assigned from comparison with the Raman profile and relative band positions observed and calculated for the isostructural compound,  $\text{YMnO}_3$ , as follows: 131( $B_{2g}$ ), 150( $B_{3g}$ ), 174( $A_g$ ), 252( $B_{1g}$ ), 279( $A_g$ ), 441( $A_g$ ) and 590( $A_g$ )  $\text{cm}^{-1}$ .

A phase transformation was observed at ca. 260 °C from the change in the Raman profile. The high temperature rhombohedral phase of  $\text{LaCrO}_3$  had four bands which are assigned as follows: 58( $E_g$ ), 161( $E_g$ ), 288( $A_{1g}$ ) and 434( $E_g, E_g$ )  $\text{cm}^{-1}$ , from comparison with the Raman profile and relative band positions observed for the isostructural compound,  $\text{NdAlO}_3$ .

The Fourier transform infrared (FTIR) spectrum of  $\text{LaCrO}_3$  showed a total of eight bands discernible at room temperature from 25 predicted modes for the orthorhombic structure. The mode assignments were determined by comparison with the Raman profile and relative band positions observed and calculated for the isostructural compound,  $\text{SmAlO}_3$ , as follows: 138( $B_{2u}$ ), 166( $B_{3u}$ ), 197( $B_{1u}$ ), 240( $B_{3u}$ ), 266( $B_{2u}$ ), 332( $B_{2u}$ ), 357( $B_{2u}$ ), 381( $B_{3u}$ ), 425( $B_{3u}$ ), 446( $B_{1u}$ ), 471( $B_{3u}$ ), 493( $B_{3u}$ ), 573( $B_{1u}$ ), 606( $B_{3u}$ ) and 670 ( $B_{1u}$ )  $\text{cm}^{-1}$ .  
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