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Vibrational spectroscopy with neutrons: recent developments.

Stewart F. Parker^{a*}, Anibal J. Ramirez-Cuesta^b, Luke Daemen^b

^a*ISIS Facility, STFC Rutherford Appleton Laboratory, Chilton, Didcot, OX11 0QX, UK*

^b*Chemical & Engineering Materials Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*

* Corresponding author.

E-mail address: stewart.parker@stfc.ac.uk (S.F. Parker).

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ABSTRACT

In this short review, we will briefly summarise the differences between INS spectroscopy and conventional infrared and Raman spectroscopies. We will illustrate these with the current state-of-the art, using C₇₀ as an example. The main focus of the article will be on the key advances in INS spectroscopy over the last ten years or so, that are driving new areas of research. The developments fall into three broad categories: (i) new sources, (ii) new and/or upgraded instrumentation and (iii) novel uses for existing instruments. For (i) we summarise the new neutron sources that are now, or will be, operating. For (ii) we show the capabilities of new or upgraded instruments. These offer unprecedented levels of sensitivity: sub-millimole quantities of hydrogen can be measured and millimole quantities of low cross section materials. Recent work on hexahalo metallates and adsorbed CO₂ is used to demonstrate what is now feasible. For (iii), instruments that were designed for studies of magnetism, are now being used for molecular spectroscopy, especially for catalysts. This is illustrated with work on CuH and methanol synthesis catalysts.

KEYWORDS

Inelastic neutron scattering; Vibrational spectroscopy; Ab initio; Infrared spectroscopy; Raman spectroscopy.

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