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Negative thermal expansion above a quantum phase transition SAHAN HANDUNKANDA, ERIN CURRY, JASON HANCOCK, Univ of Connecticut - Storrs — Strong, thermally persistent, isotropic negative thermal expansion (NTE) is unusual and has been observed in only a handful of materials. Scandium trifluoride (ScF_3) features large isotropic thermal expansion persistent over a 1000K range of temperature. More interestingly, no structural phase transition has been reported above 0.4K and it retains the simple cubic structure up to its high melting point of 1800K, which is unusual compared with other transition metal trifluorides. Here, we present a combined inelastic x-ray scattering (IXS) and x-ray diffraction study of ScF_3, which reveals some exciting features of this material. The low-energy (˜1 meV) vibrational modes corresponding to M and R points of simple cubic Brillouin zone could explain NTE in ScF3, and we find that the low temperature IXS data show a central peak which is especially strong at these points. In addition, the whole M-R branch undergoes unusual softening at low temperature. We determine that this mode softens nearly to zero energy as the temperature approaches to 0K. These signature portend an approach to a quantum phase transition of this insulating, nonmagnetic simple cubic perovskite material ScF3. The central peak, soft mode and thermal expansion could all be consequences of this incipient transition. The connections we have established in the phenomenology of ScF3 may be present in other perovskites as well as other materials that display strong NTE

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