Understanding the Dynamics of Kr@C₆₀: A Far-Infrared Vibrational Study

S. BROWN, J. CAO, J.L. MUSFELDT, University of Tennessee, N. DRAGOE, A. REVCOLEVSKI, Université Paris-Sud, Y. YOKOYAMA, S. ITO, A. TAKEDA, T. MIYAZAKI, H. TAKAGI, University of Tokyo, H. SHIMOTANI, Tohoku University, F. CIMPOESU, Institute of Physical Chemistry, Romania, K. KITAZAWA, Japan Science and Technology Agency — The C₆₀ molecule has remarkable ability to encapsulate atoms inside the hollow carbon cage. Here, we report a high-resolution far infrared spectral investigation of endohedral Kr@C₆₀. Unexpected softening of the T₁ᵤ(1) mode (∼528 cm⁻¹) and sharp peak at ∼600 cm⁻¹ have been observed throughout the temperature range of investigation. The response of Kr@C₆₀ is compared to that of pristine C₆₀, and the spectral differences are discussed in terms of local symmetry and prospects of Kr@C₆₀ as a building block for organic superconductors.

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