# Phonon propagation and thermal conductivity in the Ba8Ge40.3Au5.25 clathrate and approximant-crystal o-Al13Co4

**Pierre-François Lory** [1,2,*], S. Pailhès [5], V. Giordano [2], H. Euchner [3], Y. Grin [4], M. Baitinger [4],D Nguyen [4], M. R. Johnson [1], S. Paschen [6], H. Schober [1], C. Allio [7], E. Evteeva[7], F. Ritter [7], C. Krellner [7], Y. Sidis[8], M. de Boissieu [2,9]

[1]Institut Laue-Langevin 6, rue Jules Horowitz 38042 Grenoble, France
[2]Université Grenoble Alpes, SIMAP, Grenoble 38000 France
[3]ILM, UCBL, CNRS, UMR-5586, F-69622 Villeurbanne, Lyon, France
[4]Institute of Materials Science and Technology, TU Vienna, Vienna, Austria
[5]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany
[6]Institute of Solid State Physics, Vienna Uni. of Technology, 1040 Vienna, Austria
[7]Kristall-und Materiallabor Physikalisches Institut, Johann Wolfgang Goethe-Universität, Max-von-Laue - Straße 1, Frankfurt am Main, Germany
[8]Laboratoire Léon Brillouin, CEA Saclay, 91191 Gif sur Yvette cedex, France
(i) [9]CNRS, SIMAP, Grenoble 38000 France

[*]lory@ill.fr

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Clathrate systems are cages compounds, where guest atoms are trapped in a three dimensional network of host nanocages. A common feature of all clathrates is their low thermal conductivity (~1.3 W/m.K). This low thermal conductivity has been ascribed to the presence of the guest atom with low energy vibrational modes. However the exact mechanism at the atomic level and the way the acoustic phonon interact with the guests atoms is still a matter of debate. Different scenario have been put forward: phonon glass system where the rattling of the guest atom plays a major role [1], generalized Umklapp processes [2] and more recently a 'low energy' band pass filter due to localization and spectral weight transfer at higher energy [3-5].

We present results of a high-resolution inelastic neutron and X-rays scattering study carried out on a perfect monocrystal of the clathrate $Ba_8Ge_{40.3}Au_{5.25}$ and approximant-crystal o-$Al_{13}Co_4$. A detailed analysis of the acoustic branch has evidenced for the first time a finite lifetime of the acoustic phonon when it interacts with the low lying dispersionless excitation due to the atom in the cluster. The acoustic branch bends over severely and the acoustic phonon lifetime at this point is of the order a few picoseconds.

We have also estimated the thermal conductivity using either molecular dynamics and the Green-Kubo method, or a simple phenomenological model taking into account our INS findings.

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