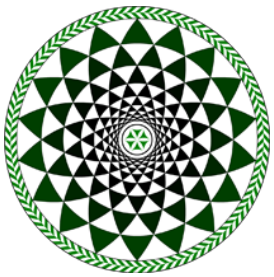

Contribution ID: **35** Type: **not specified**

Rotational Tunneling in A-methane: perturbations caused by the O₂ molecules

Friday, 10 July 2015 09:40 (30 minutes)

Neutron scattering data [1] representing rotational tunneling from CH₄ & 0.25% O₂ have been reanalyzed. They were taken at the time-of-flight spectrometer IN5 of the ILL with a wavelength of λ=13 Å. At a temperature T = 60 mK the sample was fully converted and consisted of a single spin species (A-methane). A-methane in phase II is characterized by just one tunneling transition (instead of 4): only that from A to T remains.
The width and line shape of the transition signals a significant perturbation of the methane crystal which is highly symmetric otherwise. Obviously this is the price for the admixture of the paramagnetic oxygen molecules required for the nuclear spin conversion to take place. For a better understanding the effects of replacing CH₄ at orientationally ordered sites (75%) and at disordered sites (25%) are considered separately. On concentric spherical shells around the impurity molecules the magnitude of the perturbation decreases with increasing radius. Finally a phenomenological model is used to fit the experimental data.

[1] A. Heidemann, K.J. Lushington, J.A. Morrison, K. Neumaier and W. Press; J. Chem. Phys. 81 5799 –5804 (1984)

Primary author: PRESS, Werner (IEAP, University of Kiel, Germany)

Co-author: Dr KRASNOW, Igor (IEAP, University of Kiel, Germany)

Presenter: PRESS, Werner (IEAP, University of Kiel, Germany)

Session Classification: New Ideas and Advanced Methods