Rotational Tunneling in A-methane: perturbations caused by the O_2 molecules

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Neutron scattering data [1] representing rotational tunneling from CH_4 & 0.25% O_2 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 CH_4 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;
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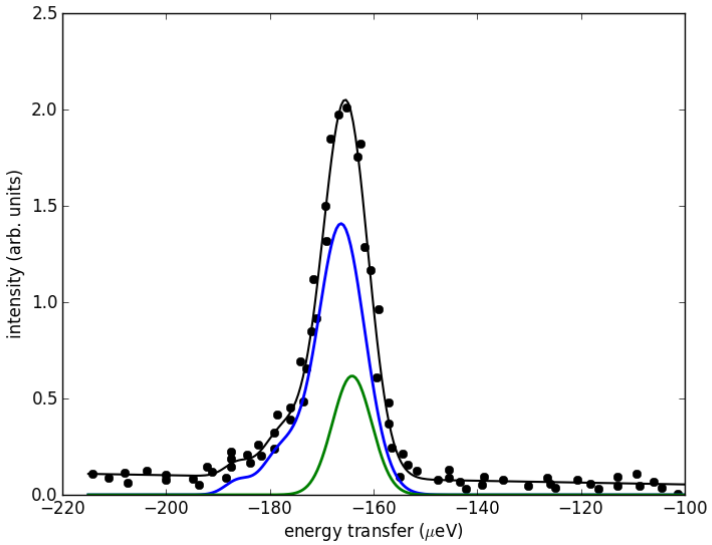

Fig. 1 Tunneling data measured with λ = 13 Å (~ 6.8 μeV, resolution at -165 μeV); the black line is a fit to the data; the blue line is the contribution with O_2 on ordered sites, the green line that with O_2 on disordered sites.