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Tunneling of the methyl protons of mesitylene trapped in a tris-(bromo-phenoxy)-triazine ”

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We have studied the transitions between the ‘rotational levels’of methyl groups of molecules isolated in cages or channels. First was studied the 1.3.5-trimethylbenzene C9H12 (mesitylene: Mes) trapped in channels of 2.4.6-tris-(bromo-phenoxy-)-1.3.5-triazine C21H12Br3N3O3 (BrPOT). The isolated guest molecules have a symmetry three, their methyl groups are equivalent, they have a tunnelling gap of 0.01 meV in the crystal. From literature the BrPOT containing Mes molecules is trigonal. INS experiments were conducted on TOFTOF and on IN5. Measurements were programmed from 1.6 K unto 50 K, with neutrons of 8.5 and 3 Å. Three pairs of tunnelling lines were recorded at 0.40, 0.20 and 0.07 meV and others above 1.4 meV. A new determination of the structure of the compound was done at 100 K: it is monoclinic with beta=118.9°, the Mes molecules are aligned in channels and inclined at 28° of the axis b. The methyl groups are now low hindered and submitted to three different hindering potentials of six-fold symmetry corresponding to slightly different environments. Results on other guests with quasi free methyl rotors will be presented.

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