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Title

(14)N quadrupole resonance and (1)H T(1) dispersion in the explosive RDX

Source

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Abstract

The explosive hexahydro-1,3,5-trinitro-s-triazine (CH(2)-N-NO(2))(3), commonly known as RDX, has been studied by (14)N NQR and (1)H NMR. NQR frequencies and relaxation times for the three v(+) and v(-) lines of the ring (14)N nuclei have been measured over the temperature range 230-330 K. The (1)H NMR T(1) dispersion has been measured for magnetic fields corresponding to the (1)H NMR frequency range of 0-5.4 MHz. The results have been interpreted as due to hindered rotation of the NO(2) group about the N-NO(2) bond with an activation energy close to 92 kJ mol(-1). Three dips in the (1)H NMR dispersion near 120, 390 and 510 kHz are assigned to the v(0), v(-) and v(+) transitions of the (14)NO(2) group. The temperature dependence of the inverse line-width parameters T(2)(+) of the three v(+) and v(-) ring nitrogen transitions between 230 and 320 K can be explained by a distribution in the torsional oscillational amplitudes of the NO(2) group about the N-NO(2) bond at crystal defects whose values are consistent with the latter being mainly edge dislocations or impurities in the samples studied. Above 310 K, the (14)N line widths are dominated by the rapid decrease in the spin-spin relaxation time T(2) due to hindered rotation of the NO(2) group. A consequence of this is that above this temperature, the (1)H T(1) values at the quadrupole dips are dominated by the spin mixing time between the (1)H Zeeman levels and the combined (1)H and (14)N spin-spin levels.