INVESTIGATIONS OF EXPLOSIVE TAGGANT VAPORS FROM ROTATIONAL SPECTROSCOPY: THE CASE OF 2,3-DIMETHYL-2,3-DINITROBUTANE

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The detection and characterization of explosives and their taggants, or of their degradation products, is a topic of crucial importance for public safety. It undoubtedly plays a key role in luggage screening and bombing scene investigations. At least two challenges need to be addressed by high-resolution spectroscopic techniques: the detection limit should be better than 1 ppb and the discriminating power should allow to unambiguously identify chemical species despite of similar properties.[1] The direct detection of classical explosives is out of reach for most spectroscopic techniques due to their extremely low vapor pressure at room temperature. Alternatively, they can be applied to the detection of explosive taggants which are intentionally added to explosives[2] or found as impurities because of the manufacturing process.

We present here the study of dimethyldinitrobutane (DMDNB), a detection taggant for explosives largely used in the United States. The microwave spectrum (2-20 GHz) was recorded with a free jet Fabry-Perot Fourier-transform microwave (FP-FTMW) spectrometer and line frequency analyses were carried out with the support of quantum chemistry calculations. The spectroscopic parameters determined for the most stable gas phase conformation include the effective quadrupole coupling constants describing the hyperfine structure arising from the two ^{14}N nuclei. The mm-wave absorption spectrum (70-110 GHz) recorded at 323 K shows features that may belong to the two other possible gas phase conformations; their analysis is in progress.[3]

[1] doi:10.3390/ma11081364, Zhang, Wei *et al.*, Recent Developments in Spectroscopic Techniques for the Detection of Explosives, Materials 11, 1364 (2018).

[2] convention Montreal, International controls to regulate plastic explosives adopted in Montreal, UN Chronicle n2, 32 (1991).

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