ROTATIONAL SPECTRUM AND QUADRUPOLE COUPLING OF 3-IODO-1,1,1-TRIFLUOROBUTANE

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We have recorded and analysed the rotational spectrum of 3-iodo-1,1,1-trifluorobutane in the 6.0–18.0 GHz region of the electromagnetic spectrum using our chirped-pulse Fourier transform microwave (CP-FTMW) spectrometer. The rotational spectrum was incredibly dense (˜1 transition every 4 MHz, on average) owing to the very low rotational constants and the quadrupolar iodine nucleus (I = 5/2) — the latter splits each rotational transition into multiple hyperfine components. However, the very large number of transitions allows accurate determination of all components of the quadrupole coupling tensor in the principal axis system. Additionally, this tensor is diagonalised into a space-fixed coordinate system to gain insight into the electric field (localised at the iodine atom) and is compared to related systems to understand the long-range effect, if any, of the three electron-withdrawing fluorine atoms on the iodine atom.