ROTATIONAL SPECTRA AND NUCLEAR QUADRUPOLE COUPLING CONSTANTS OF 4-HALOPYRAZOLES $C_3N_2H_3X$ (X = Br, I)

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The microwave spectra of the heteroaromatic molecules 4-bromopyrazole and 4-iodopyrazole have been recorded for the first time, along with their *N*-deuterated isotopologues. These species have recently been found to be useful in structural determination of proteins due to their ability to attach at a variety of binding sites.[a] The nuclear quadrupole coupling constants have been fitted, and these have been used to determine the nature of the C-X bond, and related to the strength of the halogen bonds formed by the molecules.

[a] J. D. Bauman, J. J. E. K. Harrison, and E. Arnold, *IUCrJ* 2016, 3, 51–60