Microwave spectrum of the Xe–propyne Van der Waals complex

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The microwave spectrum of the Xe-propyne Van der Waals complex has been recorded between 4—22 GHz, using a newly-developed pulsed molecular beam Fourier transform microwave spectrometer incorporating automated frequency scanning. The spectra of five isotopomers, involving ^{129}Xe, ^{131}Xe, ^{132}Xe, ^{134}Xe, and ^{136}Xe, were observed in natural abundance.
The geometry of Xe-propyne is T-shaped, comparable to that of Ar – propyne[b]. Hindered internal rotation of the methyl group in propyne splits the levels into A and E species. The A species transitions could be analysed using predictions from an on-going analysis of the infrared spectrum[c]. The microwave spectrum was analysed using a rotation-internal rotation Hamiltonian. The barrier to internal rotation V_3 was found to be $\sim 22\text{cm}^{-1}$, comparable to that of Ar-propyne.

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[c]R. O. Watts, T A. Blake, P. Muino and D. F. Eggers †, private communication