

## CHIRPED PULSE ROTATIONAL SPECTROSCOPY OF A SINGLE THUJONE+WATER SAMPLE

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Rotational spectroscopy of natural products dates over 35 years when six different species including thujone were investigated.<sup>a</sup> Nevertheless, the technique of low-resolution microwave spectroscopy employed therein allowed determination of only a single conformational parameter. Advances in sensitivity and resolution possible with supersonic expansion techniques of rotational spectroscopy made possible much more detailed studies such that, for example, the structures of first camphor,<sup>b</sup> and then of multiple clusters of camphor with water<sup>c</sup> were determined.

We revisited the rotational spectrum of the well known thujone molecule by using the chirped pulse spectrometer in Hamburg. The spectrum of a single thujone sample was recorded with an admixture of <sup>18</sup>O enriched water and was successively analysed using an array of techniques, including the AUTOFIT program,<sup>d</sup> the AABS package<sup>e</sup> and the STRFIT program.<sup>f</sup> We have, so far, been able to assign rotational transitions of  $\alpha$ -thujone,  $\beta$ -thujone, another thujone isomer, fenchone, and several thujone-water clusters in the spectrum of this single sample. Natural abundance molecular populations were sufficient to determine precise heavy atom backbones of thujone and fenchone, and H<sub>2</sub><sup>18</sup>O enrichment delivered water molecule orientations in the hydrated clusters. An overview of these results will be presented.

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<sup>a</sup>Z.Kisiel, A.C.Legon, *JACS* **100**, 8166 (1978).

<sup>b</sup>Z.Kisiel, O.Desyatnyk, E.Białkowska-Jaworska, L.Pszczółkowski, *PCCP* **5** 820 (2003).

<sup>c</sup>C.Pérez, A.Krin, A.L.Steber, J.C.López, Z.Kisiel, M.Schnell, *J.Phys.Chem.Lett.* **7** 154 (2016).

<sup>d</sup>N.A.Seifert, I.A.Finneran, C.Perez, et al. *J.Mol.Spectrosc.* **312**, 12 (2015).

<sup>e</sup>Z.Kisiel, L.Pszczółkowski, B.J.Drouin, et al. *J.Mol.Spectrosc.* **280**, 134 (2012).

<sup>f</sup>Z.Kisiel, *J.Mol.Spectrosc.* **218**, 58 (2003).