

BROADBAND ROTATIONAL SPECTROSCOPY OF CUMINOL AND ITS WATER COMPLEX

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Monoterpenoids are chemical compounds derivatives of isoprene. They are naturally produced mainly by plants and vegetations. Many of them are involved in atmospheric chemistry since they represent about 11% of the global biogenic emission, while some of them have important biological activity. Cuminol (4-isopropylbenzyl alcohol, CA), a monocyclic monoterpenoid, was found to be the main compound in Rhodiola essential oil, having a specific spicy fragrance, which emphasizes the flower scent of rose root rhizomes. It may play a role in atmospheric chemistry since it is related to the abundant atmospheric monoterpene *p*-cymene. CA is an important biological compound since it has an analgesic effect,^a and it has been found in different medicinal plants. It is also a potent insulinotropic molecule that can enhance insulin secretion.^b As biological activity is linked to the structure, it is important to characterize the conformational landscape in the gas phase. Using a combination of broadband rotational spectroscopy and theoretical calculations, one rotamer has been observed. Its identity has been confirmed by studying deuterated species enabling the determination of OH position and consequently been assigned to the lowest energy conformer. The interaction between CA and one water molecule has been also studied. Its spectrum showed tunneling effect. The splitting is associated with an internal dynamic of water inside the complex.

^aM.A. Sheikholeslami, S. Ghafghazi, S. Parvardeh, S. Koohsari, S.H. Aghajani, R. Pouriran, L.A. and Vaezi, 2021. *European Journal of Pharmacology*, 900, p.174075.

^bS.B. Patil, S.S. Takalikar, M.M. Joglekar, V. S. Haldavnekar, and A.U. Arvindekar, *British journal of nutrition*, 2013, 110, 1434-1443.