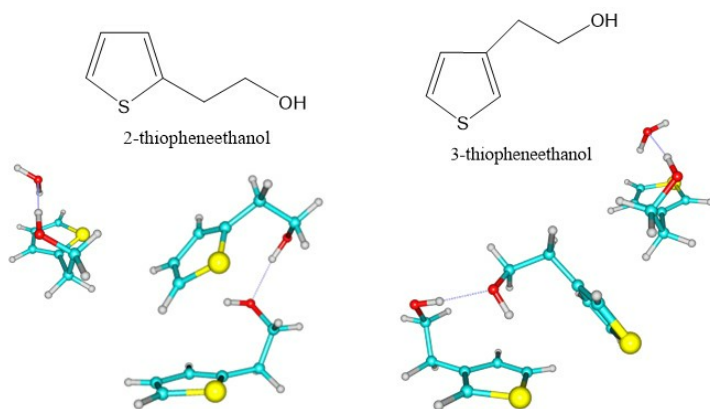


DIMERIZATION AND MICROSOLVATION OF 2- AND 3-THIOPHENEETHANOL

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We are using rotational spectroscopy to examine sulfur hydrogen bonding in a series of thiophene and furan mercapto derivatives^a, in order to compare their aggregation properties with those of the equivalent alcohols. Here we report on the dimers and monohydrates of 2-thiopheneethanol (2TE) and 3-thiopheneethanol (3TE), isolated in a jet-cooled expansion. Two isomers of (2TE)₂, three isomers of (3TE)₂ and the two monohydrates 2TE···H₂O and 3TE···H₂O were observed using chirped-pulsed and cavity Fourier transform microwave spectroscopy (2-18 GHz). The dimers are primarily bound in all cases by the stronger O-H···O interaction ($r_{O-H\cdots O}$ ca. 1.88 Å) originated by the alcohol groups. In the monohydrates water behaves as a proton acceptor, and

the spectrum shows evidence of torsional tunneling. Rotational parameters and supporting ab initio calculations will be reported.

^aM. Juanes, A. Lesarri, R. Pinacho, E. Charro, J. E. Rubio, L. Enríquez, M. Jaraíz, *Chem. Eur. J.*, **2018**, 24, 6564