Orientation of water in molecular complexes from the rotational spectra of the $H_2{}^{17}O$ species

Walther Caminati, Luca Evangelisti, Gang Feng, Qian Gou, Gloria Guidetti

Dipartimento di Chimica "G. Ciamician" dell'Universit`a, Via Selmi 2, I-40126 Bologna, Italy
Ph: 00390512099480; Fax: 00390512099456; Email: walther.caminati@unibo.it

Many molecular complexes of water with organic molecules have been investigated by rotational spectroscopy. However, in several cases the orientation of water has not been precisely determined, mainly because of the large amplitude motions of the water moiety in the complex.
Information on the orientation of water can be supplied by the quadrupole coupling constants of the ^{17}O nucleus, which nuclear spin is I = 5/2.
For this reason we analyzed the rotational spectra of several molecular complexes containing $H_2{}^{17}O$.
The results concerning the molecular complexes shown in the Figure will be presented.