

## HYDROPEROXIDES AS HYDROGEN BOND DONORS

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Hydroperoxides are formed in the atmosphere following autooxidation of a wide variety of volatile organics emitted from both natural and anthropogenic sources. This raises the question of whether they can form hydrogen bonds that facilitate aerosol formation and growth.

Using a combination of Fourier transform infrared spectroscopy, FT-IR, and *ab initio* calculations, we have compared the gas phase hydrogen bonding ability of *tert*-butylhydroperoxide (tBuOOH) to that of *tert*-butanol (tBuOH) for a series of bimolecular complexes with different acceptors. The hydrogen bond acceptor atoms studied are nitrogen, oxygen, phosphorus and sulphur. Both in terms of calculated redshifts and binding energies (BE), our results suggest that hydroperoxides are better hydrogen bond donors than the corresponding alcohols. In terms of hydrogen bond acceptor ability, we find that nitrogen is a significantly better acceptor than the other three atoms, which are of similar strength. We observe a similar trend in hydrogen bond acceptor ability with other hydrogen bond donors including methanol and dimethylamine.

