INFRARED SPECTROSCOPY OF HYDRATED NITROMETHANE ANIONS

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The hydration of molecular anions is still not as thoroughly explored as for atomic anions. We present IR spectra and quantum chemical calculations of hydrated nitromethane anions. In the monohydrate, the nitro group of the ion interacts with the water molecule via two hydrogen bonds, one from each O atom. This motif is partially conserved in the dihydrate. Adding the third water molecule results in a ring-like structure of the water ligands, each of which forms one H bond to one of the O atoms of the nitro group and another to a neighboring water ligand, reminiscent of the hydration motif of the heavier halides. Interestingly, while the methyl group is not directly involved in the interaction with the water ligands, its infrared signature is strongly affected by the changes in the intramolecular charge distribution through hydration.