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Protonated water clusters in TPC detector

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Whether intentionally or as contaminant, water is present in many gas-based detectors,owing to its low ionisation potential (12.52 eV), water is ionised both by electron impact and by charge transfer.Ionised water reacts with neutral water molecules to form H_3O^+ hydronium ions which combine with further water molecules to form large $H^+ \cdot (H_2O)_n$ clusters.Hydronium ions also combine with CO_2 molecules into mixed clusters.

These clusters are heavier and hence slower than the primary ions.This may lead to an increased dwelling time in large devices like TPCs where they increase the amount of space charge. Additionally, the signal shape will be modified. Therefore, it is important to determine the size distribution of protonated water clusters, not only at low pressure and temperature where most of the earlier experiments have been performed, but also under the conditions that prevail in detectors: atmospheric pressure and room temperature.

Here, we perform a theoretical study of the reaction
$H_3O + (H_2O)_{n-1} + H_2O \leftrightarrow H_3O + (H_2O)_n$
(n = 1-9) in the gas phase. We calculate the molecular structure and the vibration frequencies of protonated water clusters in the ground state using computational quantum mechanical modeling. The calculated equilibrium constants $K_{n-1,n}$ agree with experimental data from literature.

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