Novelty,

In the present work, theoretical investigation of the hydrotrioxy radical interaction with water, methylamine, formic acid and sulphuric acid, and subsequent hydration of the most stable 1:1 complexes are reported with emphasis on the nature of bonding, stability and essential spectroscopic properties. High-level density functional and *ab initio* calculations allowed us to describe the very first step of new particle formation in the atmosphere at the molecular level and to provide valuable information for their experimental identification. The calculations of the thermochemical parameters proved atmospheric relevance and the relative abundance of studied species.