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Exploring space chemistry: quantum spectroscopic characterization of Ng-containing molecules through machine learning algorithms.

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For a long time, space was thought to be a hostile environment characterized by extreme conditions, in which the formation of any molecular system was highly unlikely, if not impossible. However, advances in three fundamental areas of molecular astrophysics (theoretical modeling, experimental laboratories, and observational missions), as well as, their joint effort are reponsible for more than 290 molecules \[1\] have been already detected up to now. In that way, the intrigue grows with each new discovery, and the question "What comes next?" becomes more complex as the number of viable species increases. From this point of view, in the last decade, two of the most fascinated detection have been noble gas hydride cation complexes, HeH^+ and ArH^+, due to their well-known high electronic stability<a href="https://papers.ssrn.com/sol3/papers.cfm?abstract$_id = 4431879" > \22, 33, 44, [5\] < /a > .$All this has generated a great deal of interest and a desire to learn more about the interstellar-chemistry of noble gases.$
$In this vein, our main goal is to exploe trends and models using quantum chemistry computations in order to collect astrochemicall$
$ahref = "https : //www.frontiersin.org/articles/10.3389/fchem.2021.664693/full" > \46, 57, [6\] < /a > .To accomplish this, we propose a machine learning − based approach to construct new accurate potential energy surfaces fr$
aiming to understand their chemical binding and electron exchange in clusters of noble gas hydride cations.

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