Proton-driven Many-Body Interactions and Structural Organization in He$_n$H$^+$ clusters

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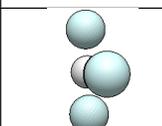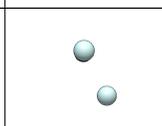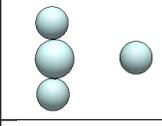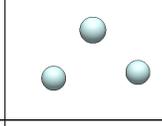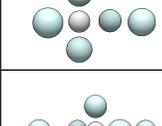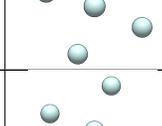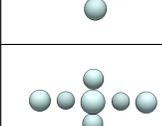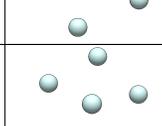[‡][2] *Departamento de Física and IUdEA, Universidad de La Laguna, 38200 Tenerife, Spain*

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SUPPLEMENTARY MATERIAL

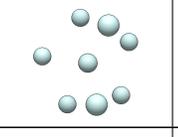Table S1: Calculated relative formation/destruction energies (in cm^{-1}) CCSD(T)/AV6Z level of theory for He$_3$H$^+$, taking to account the energy of this system like zero.

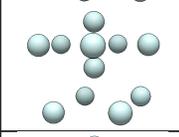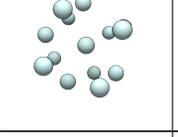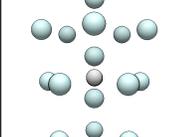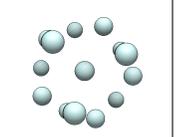| Reaction	Relative energy (cm^{-1})
He$_2$H$^+$ + He → He$_3$H$^+$	355.17
HeH$^+$ + He$_2$ → He$_3$H$^+$	4974.36
HeH$^+$ + 2He → He$_3$H$^+$	4981.58
He$_3$ + He$^+$ → He$_3$H$^+$	21429.72
He$_2$ + He + H$^+$ → He$_3$H$^+$	21437.15
3He + H$^+$ → He$_3$H$^+$	21444.38
He$_3^+$ + H → He$_3$H$^+$	88594.15
HeH + He$_2^+$ → He$_3$H$^+$	90055.51
He$_2^+$ + He + H → He$_3$H$^+$	90060.25
He$_2$ + He$^+$ + H → He$_3$H$^+$	109987.20
HeH He + He$^+$ → He$_3$H$^+$	109989.68
He$^+$ + 2He + H → He$_3$H$^+$	109994.42

Table S2: Interaction energies (in cm^{-1}) obtained from V_{4B} potential for He$_n$H$^+$ complexes, with n=3-34. The corresponding optimized structures (side and top views) are also depicted.

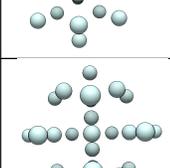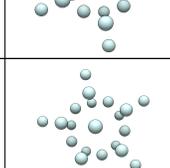|	[He$_n$H]$^+$		This work
n	Side view	Top view	V_{4B}
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4			-21788.9342
5			-22151.5468
6			-22520.6335
7			-22830.5206
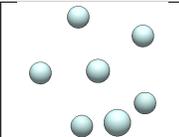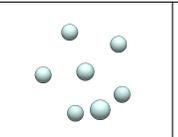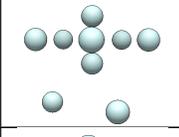
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9			-23190.1851
10			-23374.7979
11			-23552.5153
12			-23736.0593
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14			-24072.7692
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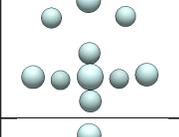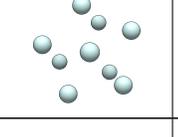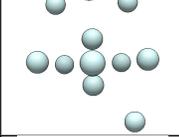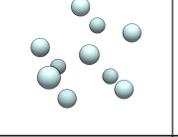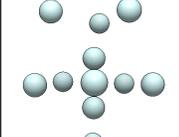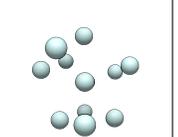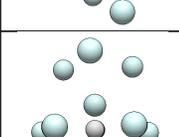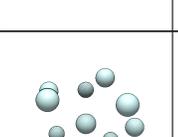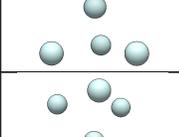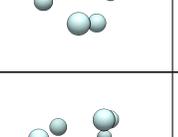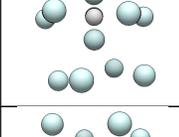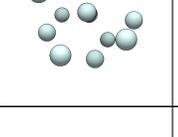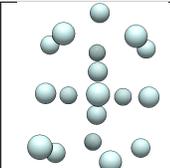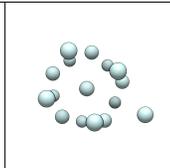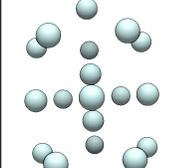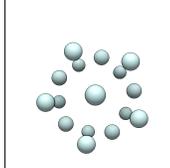
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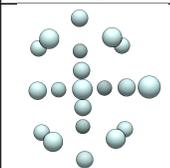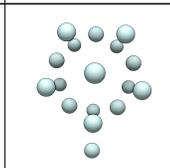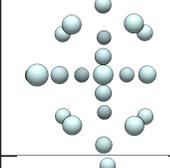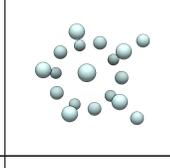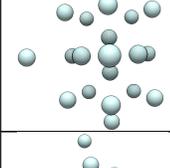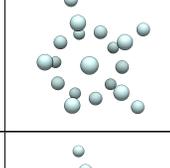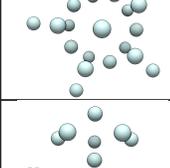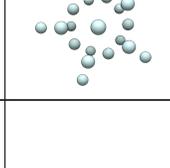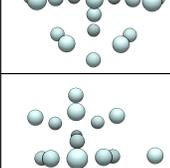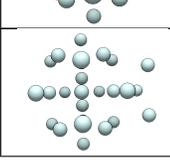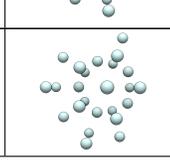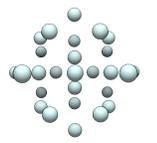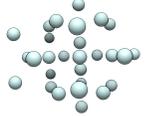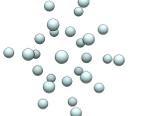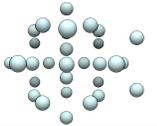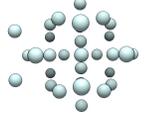
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