Higher-lying vibrational states of the $H_{5-n}D_n^+$ (n = 0-5) molecular ions

J. Sarka[a,b], C. Fábri[c], A.G. Császár[a,b]

[a] MTA-ELTE Complex Chemical Systems Research Group, H-1117 Budapest, Pázmány Péter sétány 1/A, Hungary
[b] Laboratory of Molecular Structure and Dynamics, Institute of Chemistry, Eötvös University, H-1518 Budapest 112, P.O. Box 32, Hungary
[c] Laboratory of Physical Chemistry, ETH Zürich, Vladimir-Prelog-Weg 2, 8093 Zürich, Switzerland

While the molecular ion H_5^+ and its deuterated isotopologues have considerable relevance in interstellar processes, they are also extremely interesting molecular systems on their own right. It has been shown that the rovibrational energy level structure of the astructural H_5^+ molecular ion deviates significantly from that characterizing semirigid molecules or even those showing one or two large-amplitude motions [1,2]. In the present study, a large number of higher-lying vibrational states of the various deuterated isotopologues of the H_5^+ ion are computed via variational solution of the time-independent nuclear Schrödinger equation. The latest version of the fourth-age quantum chemical program package GENIUSH [3-5] was used for this purpose. By plotting 2D cuts of the 9D wavefunctions obtained one can attempt to provide a detailed physical description of the computed vibrational states. This study further adds evidence about the unusual motions characterizing the $H_{5-n}D_n^+$ (n = 0–5) systems.

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