Higher-lying vibrational states of the H$_{5-n}$D$_n^+$ ($n = 0-5$) molecular ions

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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.