Adding exchange and multiple splitting terms to correct the long range in the H_3^+ potential surface

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The description of the long range interaction in potential energy surfaces is a hard task that has to be carefully study for every system. Particular care must be taken if the potential energy surface will be used in cold and slow collisions.

The high interest that H_3^+ produces, due to his presence in the interstellar medium[1], is evident from the large number of studies on its spectroscopy and formation by different methods (collisions, etc...). Theoretical studies require as a first step the calculation of the potential energy surfaces and in the literature there are several global potential energy surfaces for the ground[2,4] and some of the excited states[3,5] of H_3^+. However the accuracy of these surfaces is high, the intermediate and long range description is not as high as certain calculations may require, being in most of them higher than 10 cm^{-1}.

In this poster contribution we present the new terms that we are adding to the potential fit of the H_3^+ surface including the exchange splitting of the interaction energy between H and H^+, and the multipole expansion, accounting for the long range interaction between an ion (H^+) and a homonuclear neutral molecule (H_2). This expansion is added to the diagonal terms of the DIM matrix, fitted and after diagonalised to obtain the ground electronic state of H_3^+ with an accuracy lower than 1 cm^{-1} for the whole surface.

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