Study on the essential law of interaction between π bond of C2H2 and nHX(n=1 8)

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May 5, 2020

Abstract

This paper applied ab initio theoretical studies on the complex of the π bond in C2H2 and nHX(n=1 8;X=F,Cl,Br,I),formed by typical X-H···π bond complexes in geometry and energy system is described and analysed,the results demonstrated that,C2H2···nHX(n=1 8;X=F,Cl,B with increasing halogen atomic number,from HF to HI,when hydrogen halide with the same number,the complex system of X-H···π bond length and other parameters showed a periodic increase;however,with the increase of the number of hydrogen halides,the binding energy of complex with n[?]6,present in the overall increasing trend;and when n=6 reaches the maximum,in this case the π bond in C2H2 with hydrogen halide maximum capacity the limit has been reached, indicating that the π bond of C2H2···(HX)n up to six hydrogen halide molecules interactions to the formation of X-H···π bond complexes,that is to say X-H···π bond in C2H2···nHX complex have saturation property,and in the n=6 reach saturation state.

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2019-Jie Yang-C2H2-nHX-0616 - yingwen.doc available at https://authorea.com/users/286746/articles/411182-study-on-the-essential-law-of-interaction-between-%CF%80-bond-of-c2h2-and-nhx-n-1-8

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