

Hydrogen bonds in inorganic crystals: a microscopic study on the valence electron distribution of hydrogen in O–H...O systems.

Autorzy

Fang Zhang

K. Li

Henryk Ratajczak

D. Xue

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From the chemical bond viewpoint, we scrutinized the valence electron distribution of hydrogen in O–H...O systems in inorganic crystals. The influence of different crystalline environments on the original O–H bond lengths d_0 of O–H...O hydrogen bonds was quantitatively expressed by a function of d_0 versus the length of the constituent bonds. It is clearly shown that the valence electron distribution of hydrogen is affected evidently by the detailed environments of the O–H...O systems and the results agree well with the bond valence sum rule. Furthermore, the shortest O–H length in crystals is predicted to be 0.806 Å which is consistent with the value of 0.798 Å detected by neutron diffraction measurements. The current work establishes a bridge between structure and microscopic properties of hydrogen bonds, which can give us a useful clue to the utilization of hydrogen bonds in the design of inorganic functional materials.

Słowa kluczowe

Hydrogen bond, Valence electron distribution, Inorganic crystal materials, Original bond length

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