

## Nature of Brønsted acid-noble atom contacts: a reevaluation of hydrogen bonding criteria.

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### Streszczenie

Xenon atoms interact weakly and reversibly with different molecular systems and human body. In this report, we consider their participation in hydrogen bonding in relation to analogous interactions of Ne, Ar, and Kr. Acid–noble atom dimers,  $A\cdots H\cdots Rg$ , are examined by the quantum theory of atoms in molecules and the results are discussed using several independent parameters. Different factors of this complexation are recognized: (i) the AH acidity and the Rg basicity, (ii) the AH structure, (iii) the electronegativities of atoms A and Rg, and (iv) the charge transfer from Rg to the complex critical point and to the acidic H atom.  $A\cdots H\cdots Ne$  contacts are qualitatively different from the remaining complexes. Koch and Popelier's criteria of hydrogen bonding, developed for classic complexes, are usually fulfilled for these very weak systems with one main exception: the charge on the acidic H increases upon the complexation to bigger Rg atoms.

### Adres publiczny

<http://dx.doi.org/10.1002/qua.24612>

### Strona internetowa wydawcy

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