

## The hypervalent $\text{PF}_4\text{H}$ species dimer: a system with double blue-shifted $\text{P}-\text{H}\cdots\text{F}$ hydrogen bonding?.

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### Streszczenie

The hypervalent  $\text{PF}_4\text{H}$  species dimer has been studied using second-order perturbation theory and coupled-cluster methods with augmented correlation-consistent basis sets up to truncated quadruple-zeta. The dimer involving two  $\text{P}-\text{H}\cdots\text{F}$  contacts serves a model of weak interaction between  $\text{PF}_4\text{H}$  molecules in the crystal. We found dimer structures of  $C_{1s}$  and  $C_i$  symmetry with interaction energy of the order of -2.5 kcal/mol. SAPT (symmetry-adapted perturbation theory) energy decomposition scheme reveals major electrostatic, polarization and dispersion stabilizing contributions. We are not conclusive as to the presence of improper H-bonding in this complex.

### Adres publiczny

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### Strona internetowa wydawcy

<http://www.elsevier.com>