

# The spin-spin coupling constants transmitted through van der Waals interactions

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## Abstract

The  $^{19}\text{F}$ - $^1\text{H}$  coupling constants were calculated on the MCSCF level in several systems, ranging from covalently bonded HF, hydrogen bonded  $\text{FHF}^-$  and  $(\text{HF})_2$  complexes to weak van der Waals complex  $\text{CH}_4 - \text{HF}$ . The sign of the  $^{19}\text{F}$ - $^1\text{H}$  coupling varies in this sequence, and its absolute value decreases. Still, it is sizable even for  $\text{CH}_4 - \text{HF}$ . The distance dependence of  $^{19}\text{F}$ - $^1\text{H}$  coupling is essentially the same in all systems under study, and the calculations for  $\text{FHF}^-$  with distorted geometry suggest that the value of  $^{19}\text{F}$ - $^1\text{H}$  coupling is determined mainly by molecular geometry.  $^{19}\text{F}$ - $^{19}\text{F}$  intermolecular coupling in  $(\text{HF})_2$  is substantial but has the opposite sign to that in  $\text{FHF}^-$  and its counterpart in  $(\text{H}_2\text{O})_2$ . The agreement of the couplings calculated for HF and  $\text{FHF}^-$  with experiment suggests that the other results are also reliable.