

Aurophilic attraction: The additivity and the combination with hydrogen bonds

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The coexistence of gold-gold contacts and hydrogen bonding is studied in the model system $[\text{H}_2\text{P}(\text{OH})\text{AuCl}]_2$ and $[\text{H}_2\text{P}(\text{OH})\text{AuPH}_2(\text{O})]_2$. The two interactions are found to be comparable. The possible non-additivity of the aurophilic, Au(I)-Au(I) interaction is studied at MP2 level for the pentagonal $[\text{Au}(\text{SH})_2(\text{AuSH})_5]^-$ and hexagonal $[\text{Au}(\text{SH})_2(\text{AuSH})_6]^-$ clusters. The possibilities of 'mechanical cooperativity' between different aurophilic attractions and of Au...S attractions are also considered. © 2003 Published by Elsevier Science B.V.