The Significance of C-H···π(metalloaromatic) Interactions in Stabilising Crystal Structures

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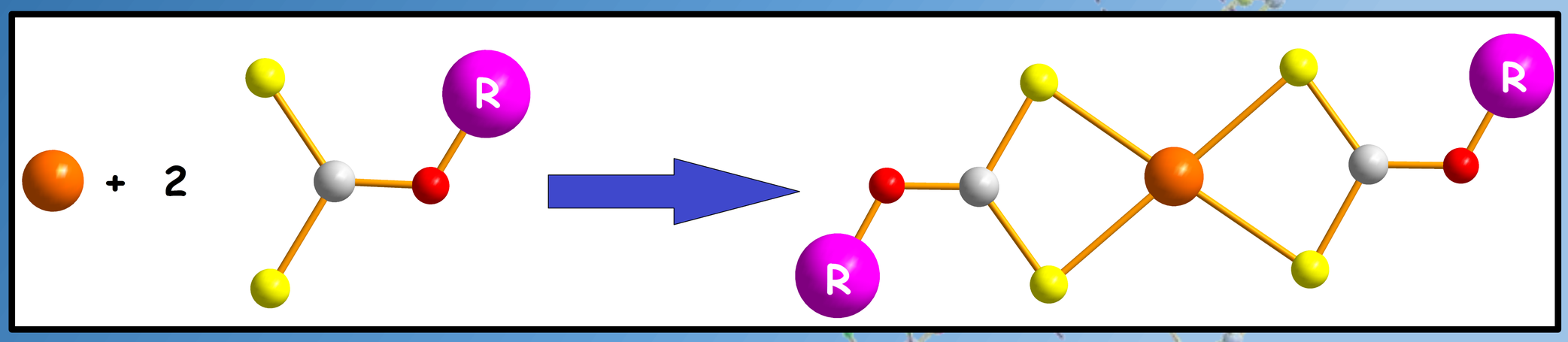
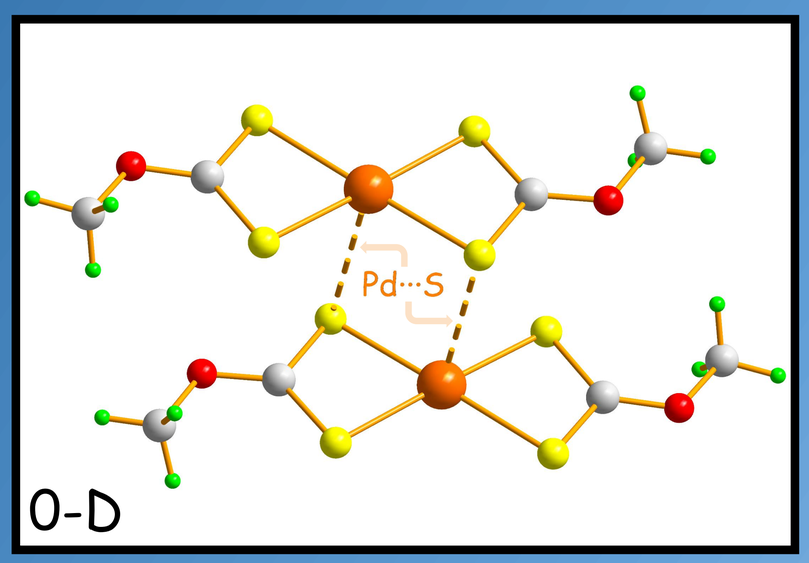
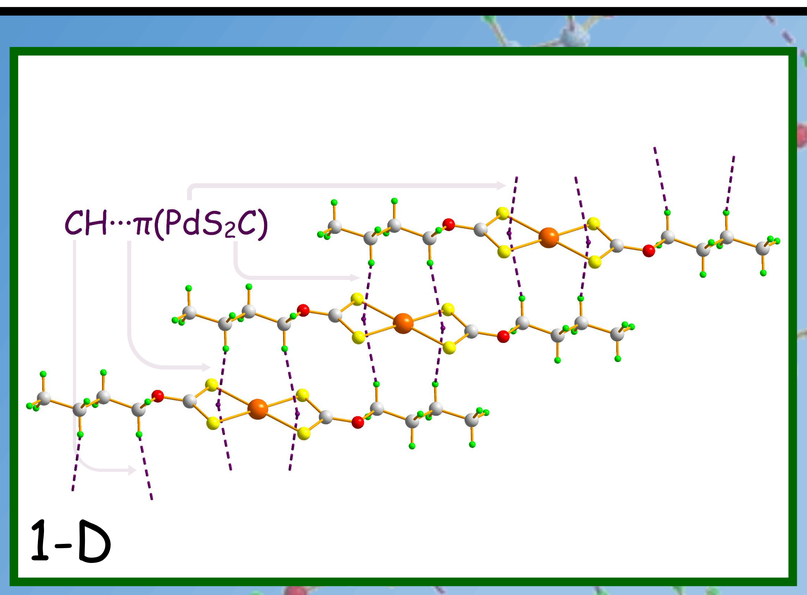
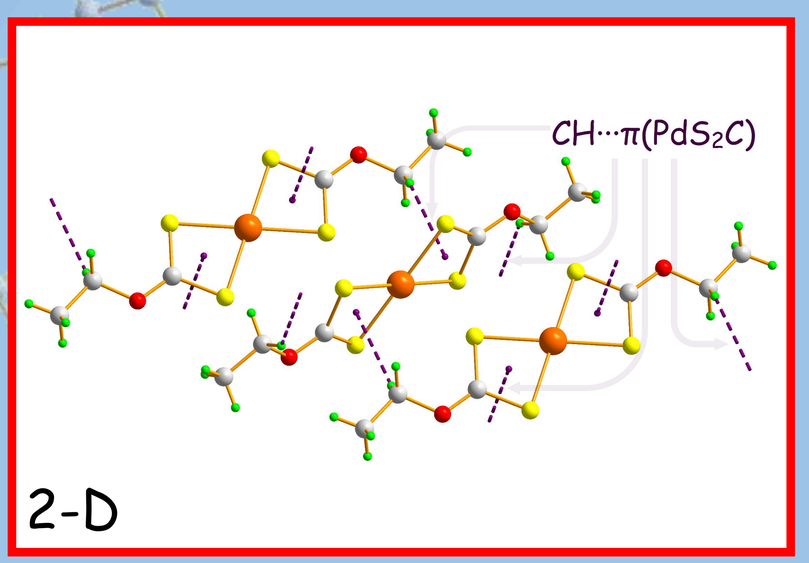
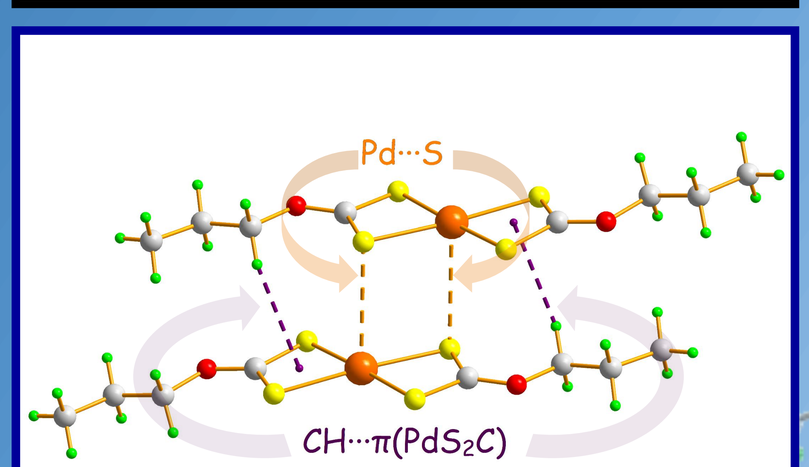
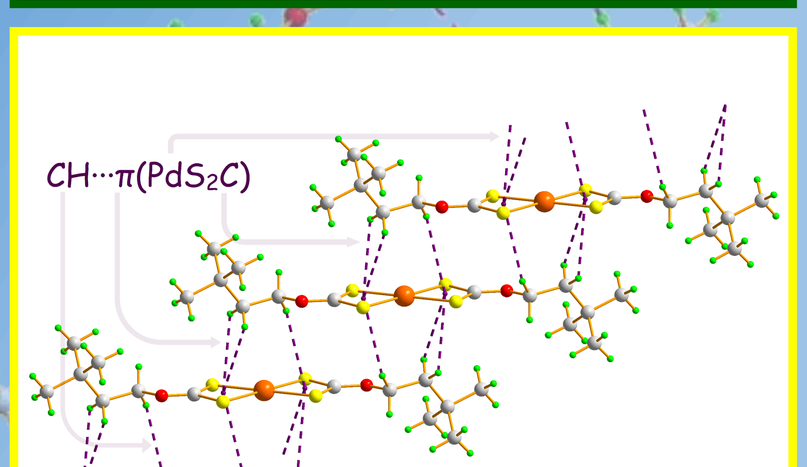


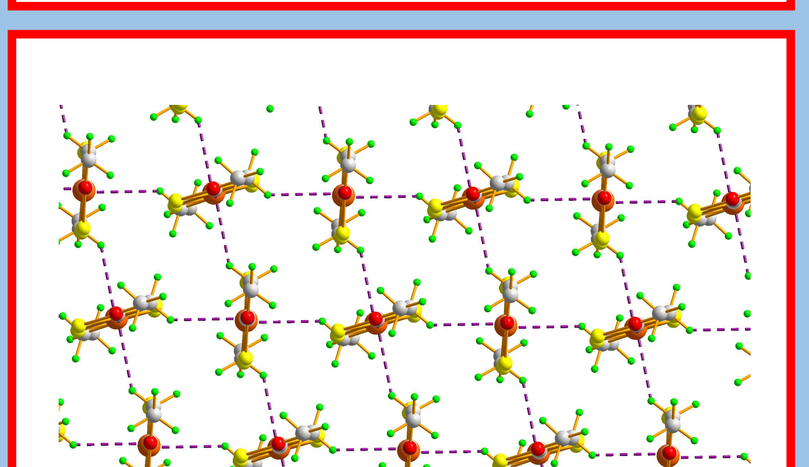


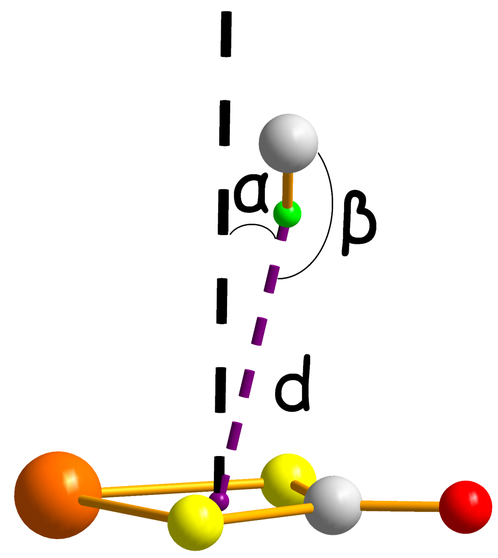






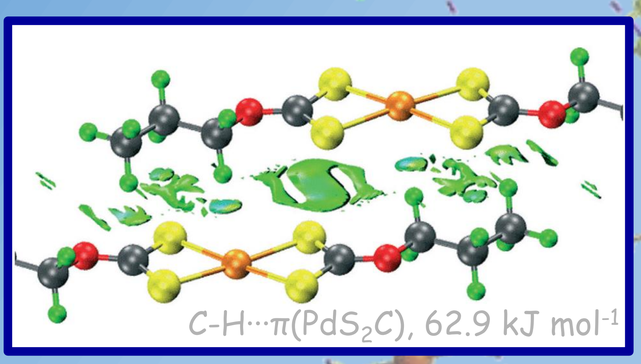


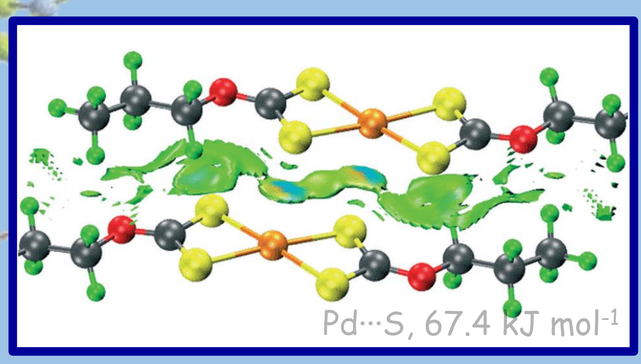


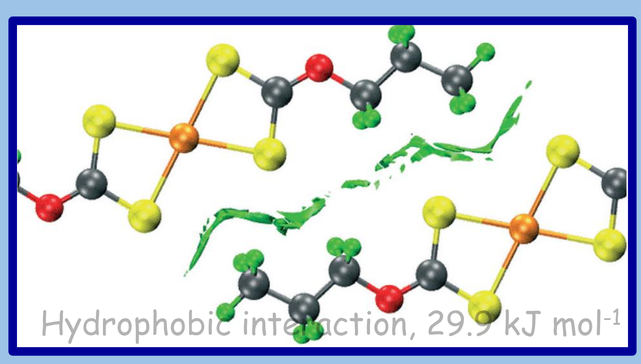


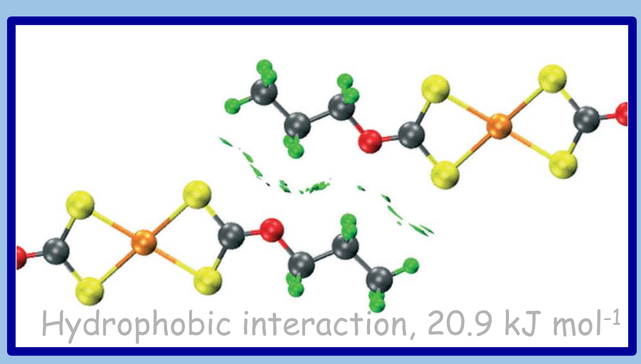
	Reference	Observation
CH···π(PdS2C)	α > 20°, 110° ≤ β ≤ 180°, 2.4Å ≤ d ≤ 3.6Å	α = 14.26°, β = 143.43°, d = 2.91Å
Pd···S	d ≤ 3.43Å (1.63Å + 1.80Å)	d = 3.37Å

E. R. T. Tiekink and J. Zukerman-Schpector Chem. Commun., 2011, 47, 6623-6625


C-H···π(PdS2C), 62.9 kJ mol-1


Pd···S, 67.4 kJ mol-1


Hydrophobic interaction, 29.9 kJ mol-1


Hydrophobic interaction, 20.9 kJ mol-1

Conclusion: 11 out of 12 synthesised Palladium Xanthates show the presence of C-H···π(PdS2C) interactions. Calculation Prove that the interaction is one of the main factors contributing to the crystal packing with comparative strength as the Pd···S dimerisation interaction.

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