

Really, how significant is hydrogen-bonding in supramolecular association in molecular crystals?

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Acad. Ionel Haiduc at the age of 80 - Cluj 2017

Molecular packing

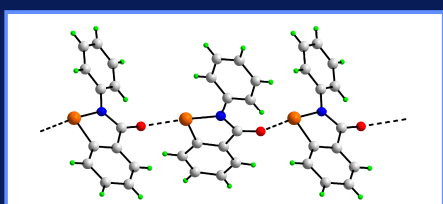
Well known...

Hydrogen bonding
Halogen bonding

"Emerging"

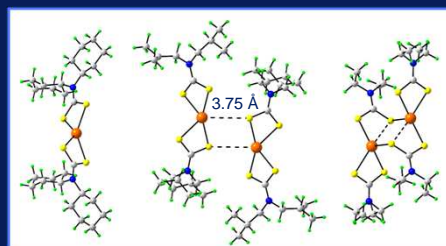
Secondary bonding
M...M interactions
M...H interactions
Interactions involving chelate rings

Tetrel, Pnictogen and Chalcogen Secondary Bonding



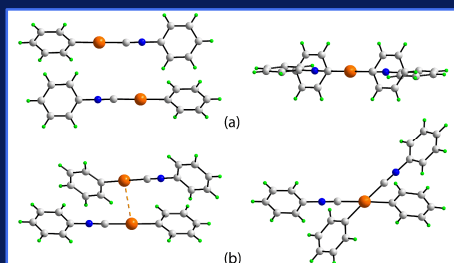
Se...O in Ebselen®
polar gap, σ -hole; ~8 kcal/mol

Steric effects and secondary bonding



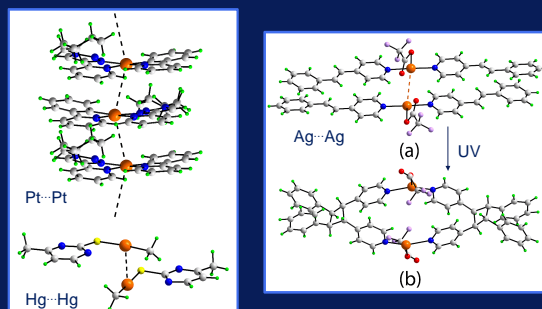
"Hg(S₂CNR₂)₂"
Sum of the van der Waals radii for Hg and S = 3.35 Å

Aurophilic (Au-Au) interactions

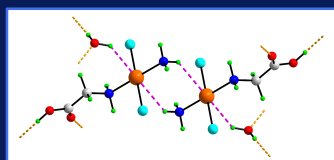


Polymorphs of PhAuC≡NPh
(a) to (b) touch of a needle / mechanical grinding

Heterometallophilic (M-M') interactions

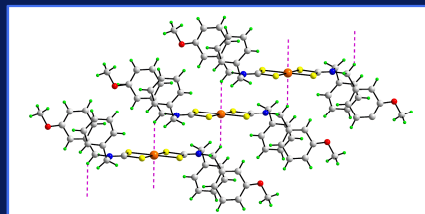


Metal...hydrogen interactions as supramolecular synthons



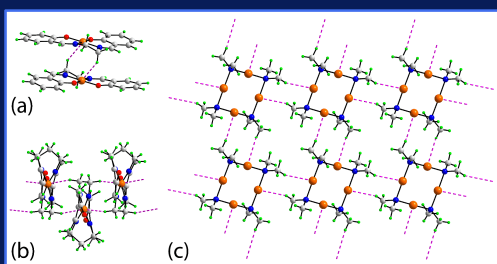
Pt...H-N and Pt...H-O hydrogen bonding in trans-[PtCl₂(NH₃)(N-glycine)]

Metal...hydrogen interactions as supramolecular synthons



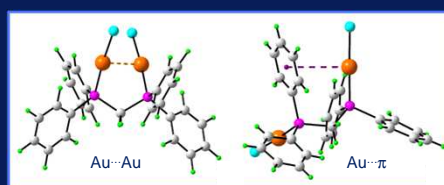
Ni...H interactions in Ni(S₂CNR')₂

Metal...hydrogen interactions as supramolecular synthons



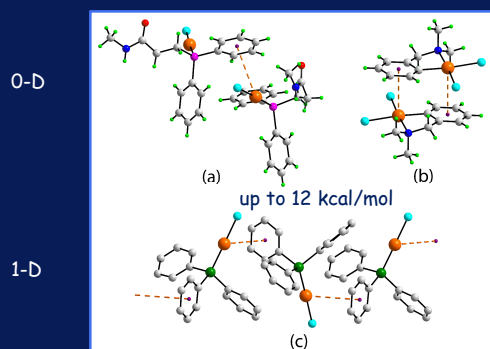
Architectures sustained by {...HCNM}₂ synthons

Au...π(arene) interactions

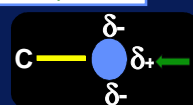
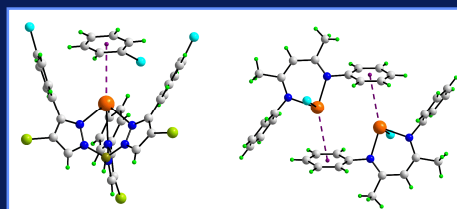


Polymorphs of (Ph₂PCH₂PPh₂)(AuCl)₂

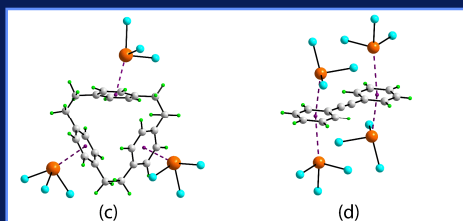
Intermolecular Au...π(arene) interactions



Intermolecular M(lp)...π(arene) interactions

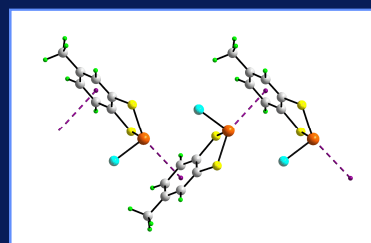


Intermolecular $M(lp) \cdots \pi(\text{arene})$ interactions

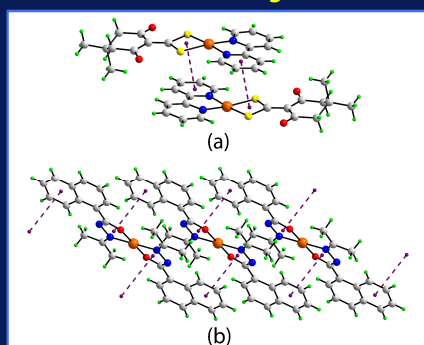


up to 10 kcal/mol

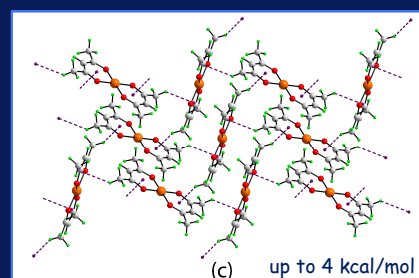
Intermolecular $M(lp) \cdots \pi(\text{arene})$ interactions



Intermolecular interactions involving chelate rings

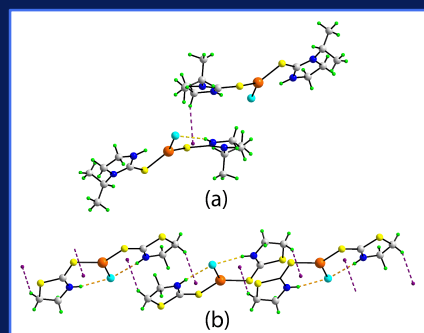


Intermolecular interactions involving chelate rings



up to 4 kcal/mol

Intermolecular interactions involving quasi-chelate rings



Conclusions

More than hydrogen bonding

Energies of "emerging" interactions similar

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Fortuna Eruditis Favet ("Fortune favours the prepared mind")

Announcement



7th Asian Conference on Coordination Chemistry (ACCC7)
22-26 July 2019 / Kuala Lumpur, Malaysia
(Organised by Institut Kimia Malaysia)

You are welcome to visit the conference's website at www.accc7.org.my for updates on ACCC7 or you can email us at accc7@ikm.org.my for further details.