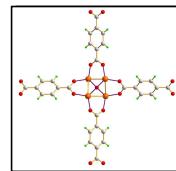




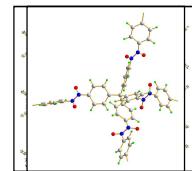
EXPLORING C-H...METALLOAROMATIC INTERACTIONS

YEE SENG TAN
RESEARCH CENTRE FOR CRYSTALLINE MATERIALS
SUNWAY UNIVERSITY
MALAYSIA

Crystal Formation (Primary Bonding)

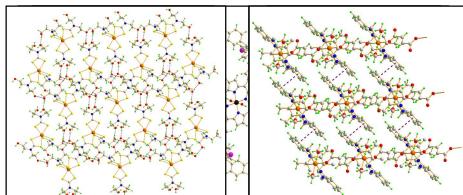


REFCODE: SHAYIK



VIHFID

Crystal Formation (Secondary Bonding)



REFCODE: RUGSIV01 DUKFOG EGODEL

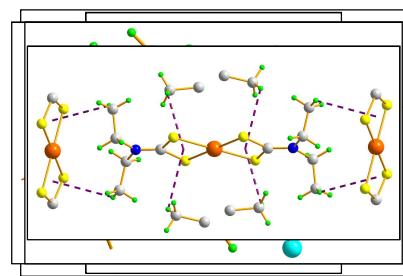
Crystal Formation (Secondary Bonding)

REFCODE:

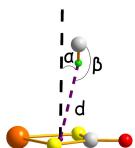
RUGSIV01

REFCODE: RUGSIV01

EGODEL



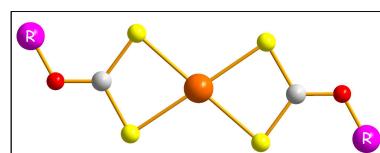
Introduction, C-H...Metalloaromatic Interactions



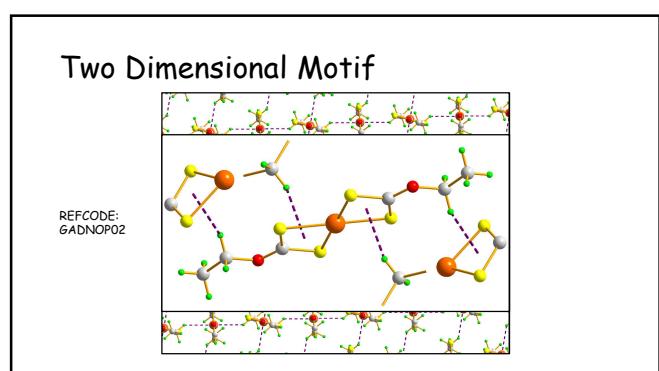
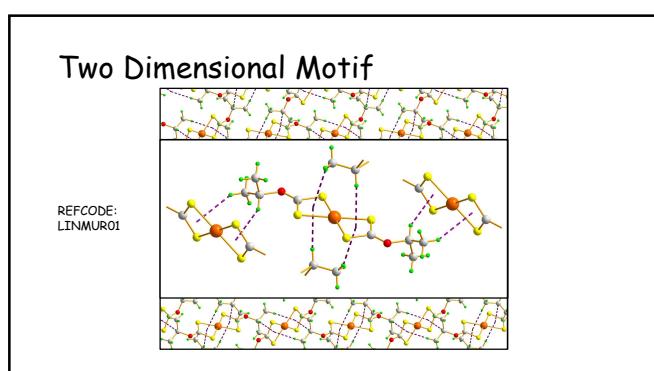
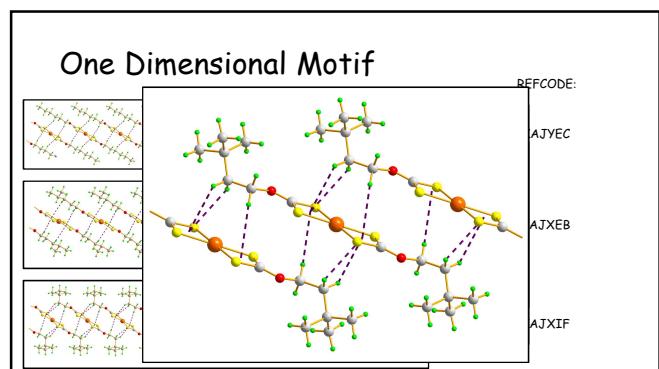
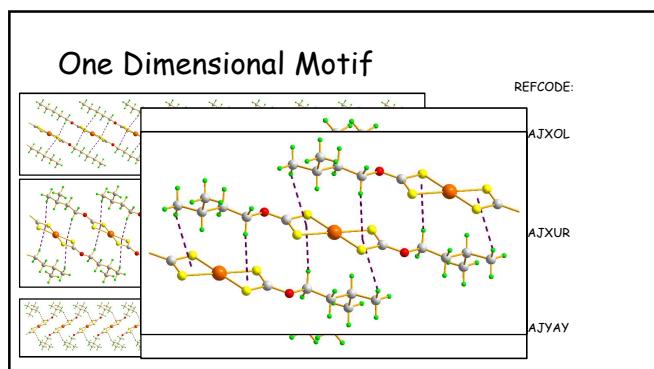
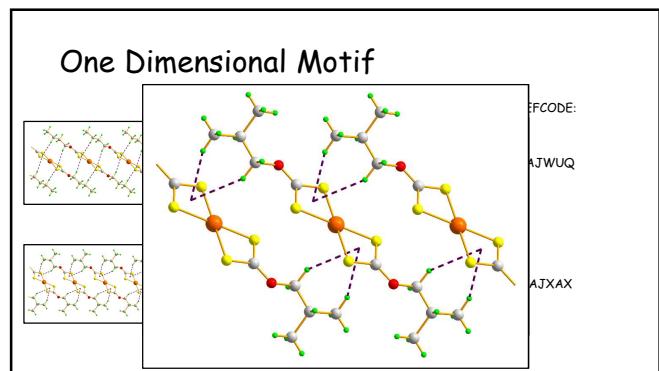
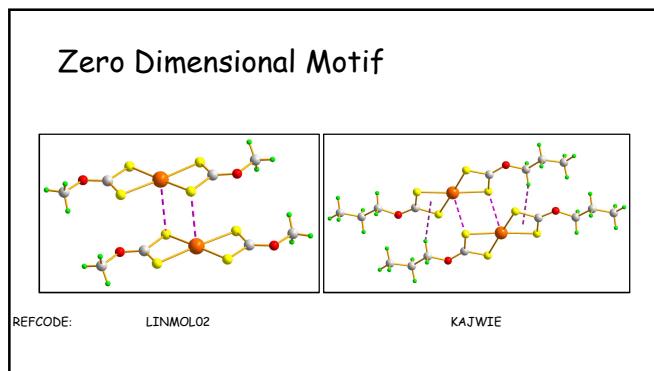
- C-H ... π (Chelate)
 - $\alpha < 20^\circ$
 - $110^\circ \leq \beta \leq 180^\circ$
 - $2.4 \text{ \AA} \leq d \leq 3.6 \text{ \AA}$

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

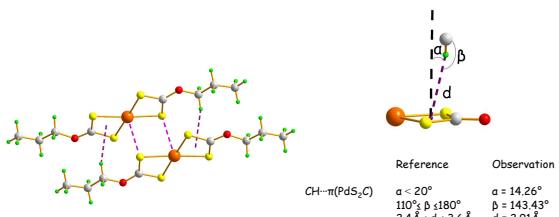
Palladium(II) Xanthate



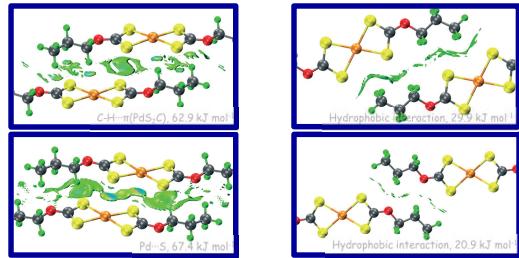
R= Me, Et, n-Pr, i-Pr, n-Bu, i-Bu, n-Pent, i-Pent, neo-Pent, n-Hx, i-Hx, neo-Hx



Computational Calculation



Stabilising Energy



Conclusion

- 12 compounds
 - Crystallographically studied
- $\text{C-H}\cdots\pi(\text{metalloaromatic})$
 - 11/12 Compounds
- Strength of the $\text{C-H}\cdots\pi(\text{metalloaromatic})$ interaction
 - Similar with Coordination Bond Pd-S
- Emerging but non-common focus interaction
 - Important in Crystal System

Acknowledgment

- Sunway University
- ACCC6 Organising Committee
- Professor Dr Edward R. T. Tiekkink
- Dr Siti Nadiah Binti Abdul Halim
- Dr Alberto Otero-de-la-Roza



After ACCC6 in Melbourne???????



ACCC7 at Kuala Lumpur, Malaysia in 2019



Photo taken from www.tourism.gov.my

ACCC7 at Kuala Lumpur, Malaysia in 2019



ACCC7 at Kuala Lumpur, Malaysia in 2019

