EXPLORING C-H∙∙∙METALLOAROMATIC INTERACTIONS

YEE SENG TAN
RESEARCH CENTRE FOR CRYSTALLINE MATERIALS
SUNWAY UNIVERSITY
MALAYSIA

Crystal Formation (Primary Bonding)

Crystal Formation (Secondary Bonding)

Introduction, C-H∙∙∙Metalloaromatic Interactions

• C-H ∙∙∙π(Chelate)
• α < 20°
• 110° ≤ β ≤ 180°
• 2.4 Å ≤ d ≤ 3.6 Å


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
Zero Dimensional Motif

One Dimensional Motif

One Dimensional Motif

Two Dimensional Motif

Two Dimensional Motif
Computational Calculation

Reference: Reference Observation

CH∙∙∙π(PdS₂C) α < 20° α = 14.26°

110° ≤ β ≤ 180° β = 143.43°

2.4Å ≤ d ≤ 3.6Å d = 2.91Å

Stabilising Energy

Conclusion

- 12 compounds
- Crystallographically studied
- C-H∙∙∙π(metalloaromatic)
- 11/12 Compounds
- Strength of the C-H∙∙∙π(metalloaromatic) interaction
  - Similar with Coordination Bond Pd∙∙∙S
- Emerging but non-common focus interaction
  - Important in Crystal System

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After ACCC6 in Melbourne???????

ACCC7 at Kuala Lumpur, Malaysia in 2019
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