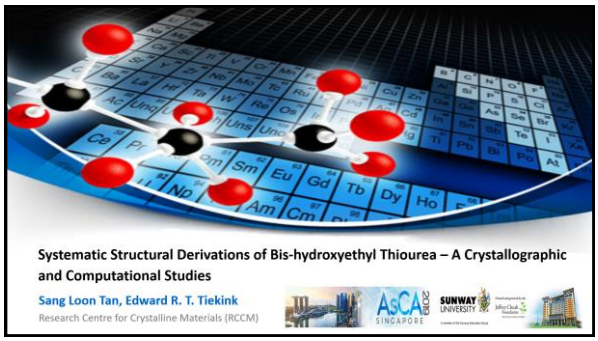
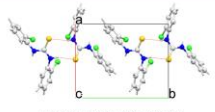


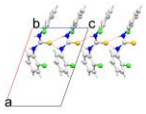
Systematic Structural Derivations of Bis-hydroxyethyl Thiourea – A Crystallographic and Computational Studies

Sang Loon Tan, Edward R. T. Tiekink
Research Centre for Crystalline Materials (RCCM)

Intermolecular Interaction and Crystal Packing



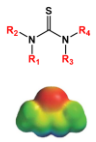
Acta Cryst. (1996). C52, 134-136



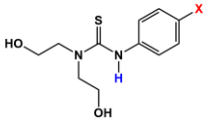
Acta Cryst. (2011). E67, o2965

Intermolecular interaction ⇄ Crystal packing

Bishydroxyethyl Thiourea Derivatives



Chem. Commun. (2008), 295–307

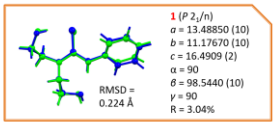


(1) 4-H
(2) 4-CH_3
(3) 4-Cl
(4) 4-NO_2

Objectives of Study:

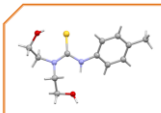
1. To study the differences in the molecular interactions and crystal packing of the of the four thiourea derivatives
2. To rationalize the crystallographic differences through computational approach

Crystal Structures

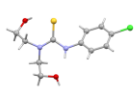


RMSD = 0.224 Å

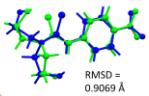
1 ($P\,2_1/n$)
a = 13.48850 (10)
b = 11.17670 (10)
c = 16.4909 (2)
α = 90
β = 98.5440 (10)
γ = 90
R = 3.04%



2 ($P\,2_1/n$)
a = 7.0472 (2)
b = 10.7489 (2)
c = 16.9533 (4)
α = 90
β = 99.109 (2)
γ = 90
R = 2.91%



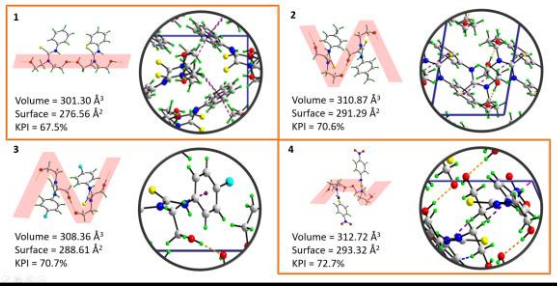
3 ($P\,2_1/n$)
a = 7.1366 (2)
b = 10.7767 (3)
c = 16.6259 (4)
α = 90
β = 100.221 (2)
γ = 90
R = 3.08%



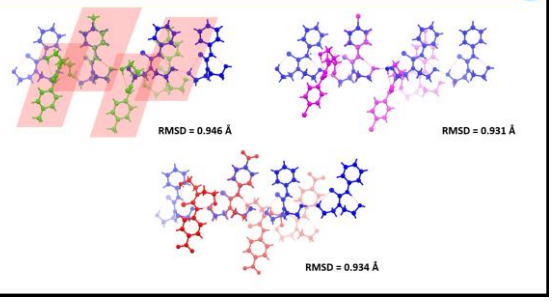
RMSD = 0.9069 Å

4 (P -1)
a = 10.8235 (5)
b = 11.2124 (5)
c = 12.3443 (5)
α = 90.050 (3)
β = 108.737 (4)
γ = 114.559 (4)
R = 4.08%

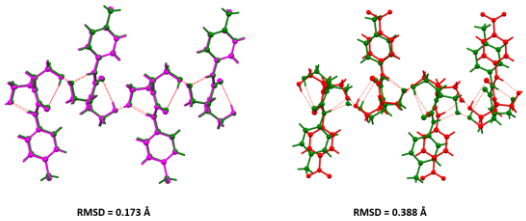
Crystal Packing



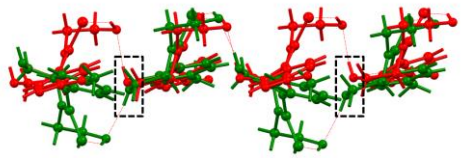
Comparison of Crystal Packing between 1 and 2, 1 and 3, 1 and 4



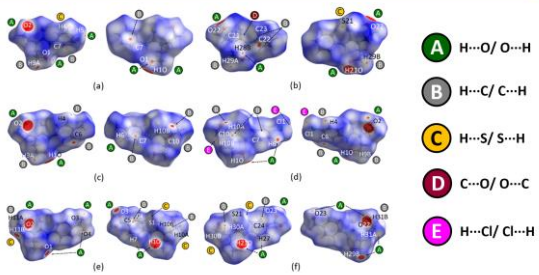
Comparison of Crystal Packing between 2 and 3, 2 and 4



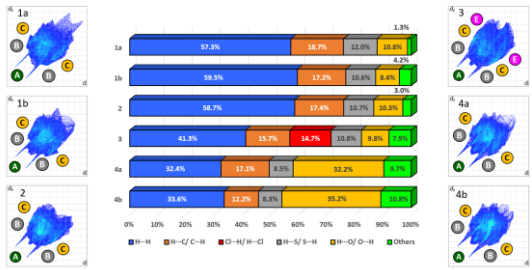
Comparison of Crystal Packing between 2 and 4



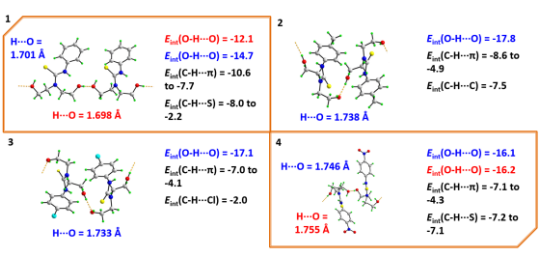
Hirshfeld Surface Analysis



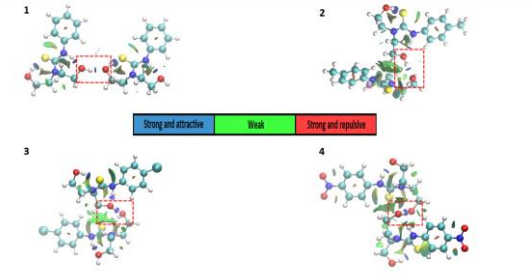
Hirshfeld Surface Analysis



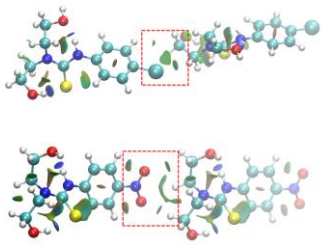
Interaction Energy (kcal/mol)



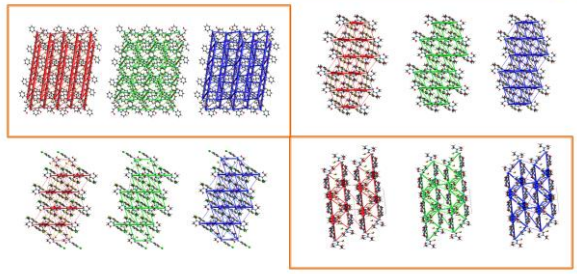
Non-Covalent Interaction Plots (NCIPlot)



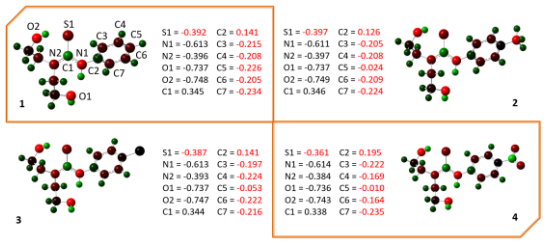
Non-Covalent Interaction Plots (NCIPlot)



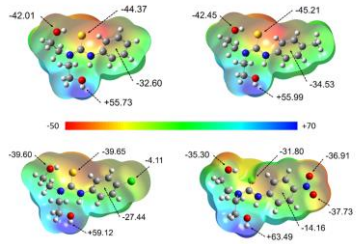
Energy Framework



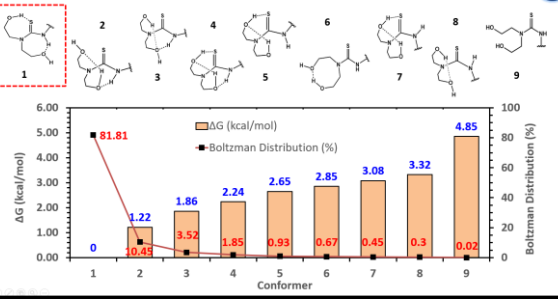
Natural Population Analysis



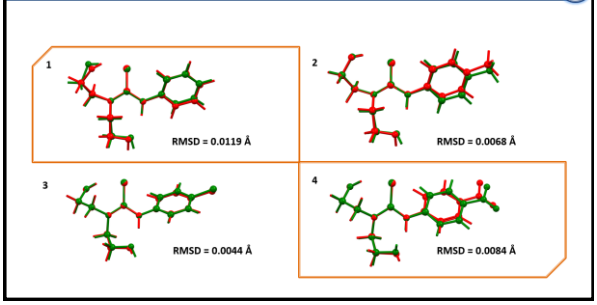
Electrostatic Potential Mapping (ESP)



Conformer Distribution



Comparison between Crystal and Optimized Structures



Conclusions

- Introduction of different substituents in the 4-phenyl position lead to crystal packings which are very different from the parent structure.
- Minor differences in intermolecular interactions with small energy window lead to similar crystal packing.
- Presence of complementary interactions help in diversify crystal packing.

Formation of Crystal Structure