Electronic Supplementary Material (ESI) for New Journal of Chemistry

Theoretical investigation on the nature of substituted benzene···AuX interactions: covalent or noncovalent?

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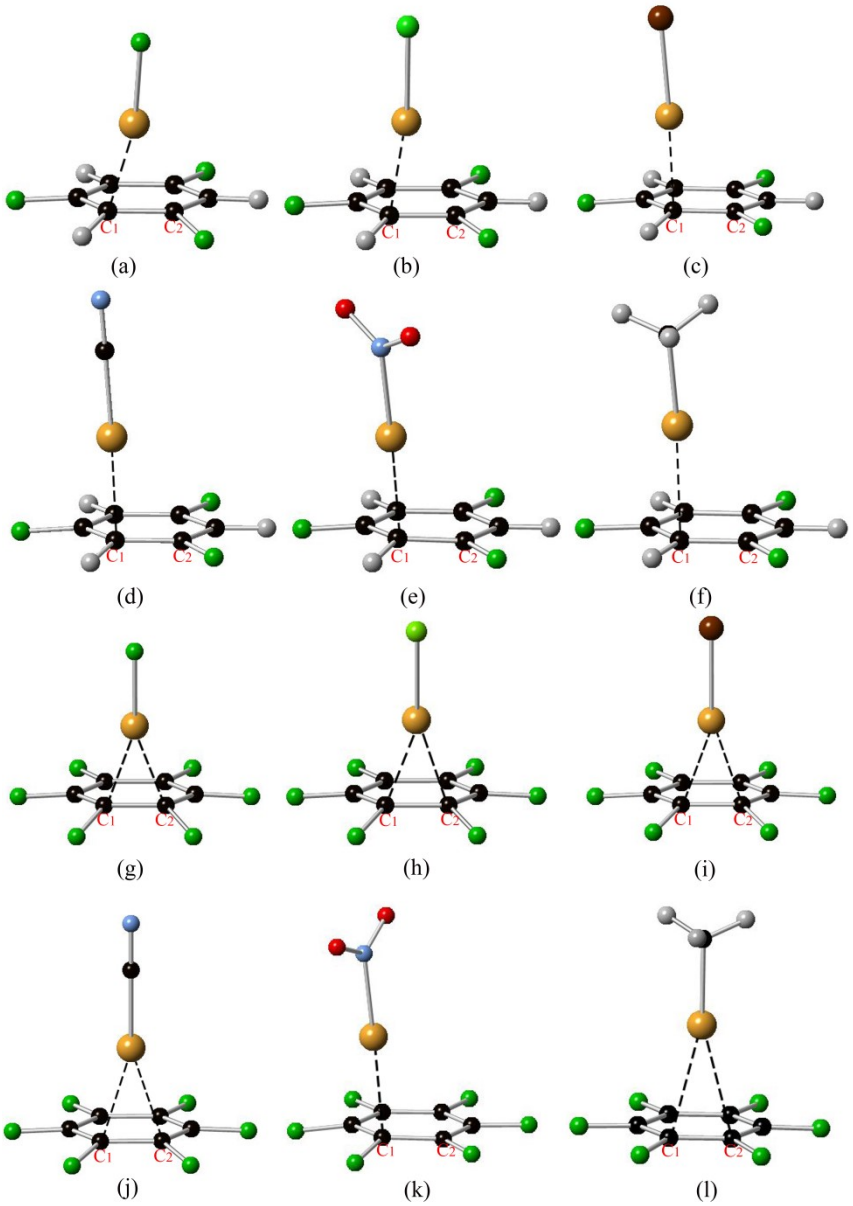
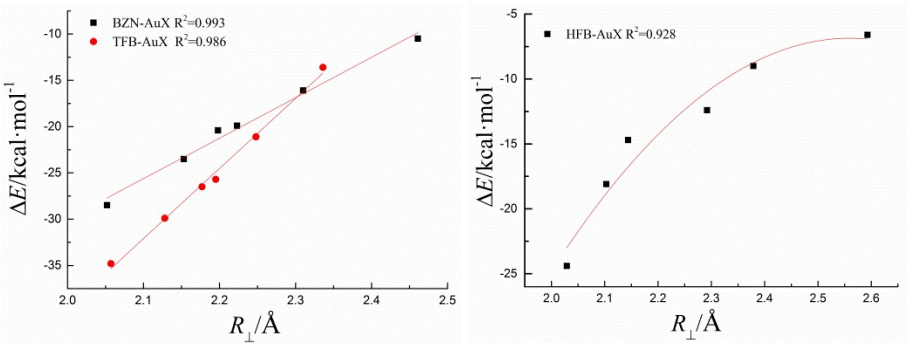
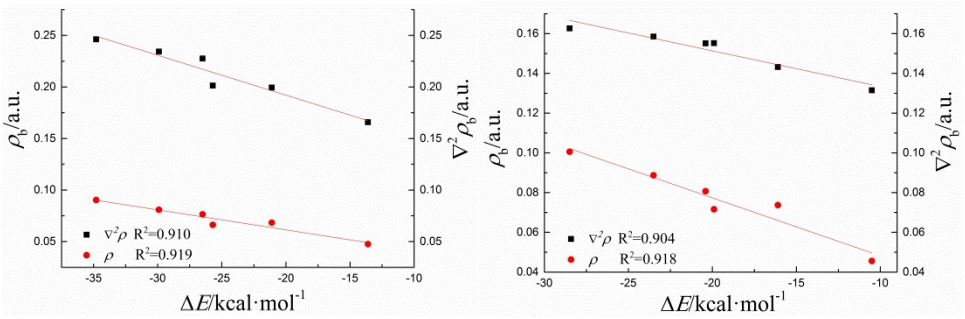


Figure S1 Optimized geometries of the complexes: (a) TFB···AuF, (b) TFB···AuCl, (c) TFB ···AuBr, (d) TFB ···AuCN, (e) TFB ···$AuNO_2$, (f) TFB ···$AuCH_3$, (g) HFB···AuF, (h)HFB···AuCl, (i) HFB···AuBr, (j) HFB ···AuCN, (k) HFB ···$AuNO_2$, (l) HFB ···$AuCH_3$

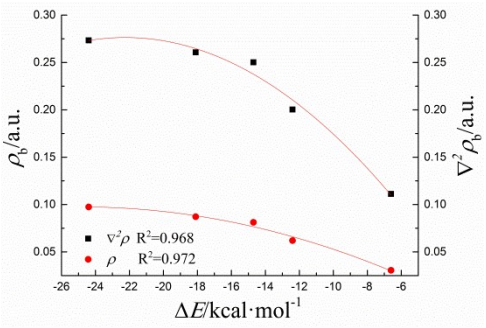


(a) (b)

Fig. S2 Relationships between binding energies ΔE and equilibrium distance $R_\perp$ for the π···AuX complexes (a) BZN···AuX and TFB···AuX (b) HFB···AuX



(a) (b)



(c)

Fig. S3 Relationships between binding energies ΔE and electron density ρ_b or its Laplacian $\nabla^2\rho_b$ at the C···Au BCPs or RCPs in the complexes (a) BZN···AuX (b) TFB···AuX (c) HFB···AuX

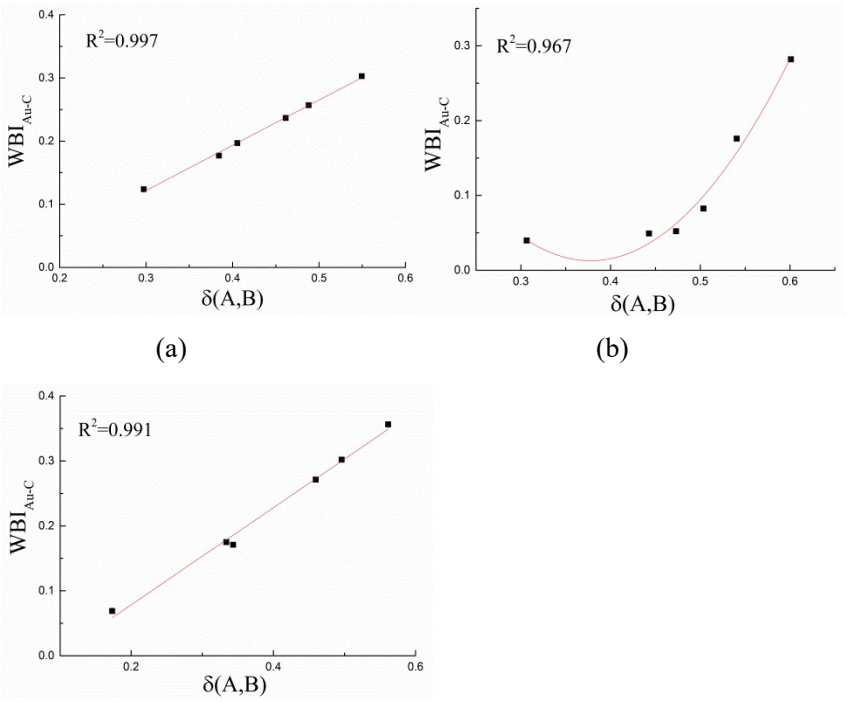


Fig. S4 Relationships between delocalization index δ(A, B) and Wiberg bond index $WBI_{Au\text{-}C}$ for the complexes (a) BZN···AuX (b) TFB···AuX (c) HFB···AuX

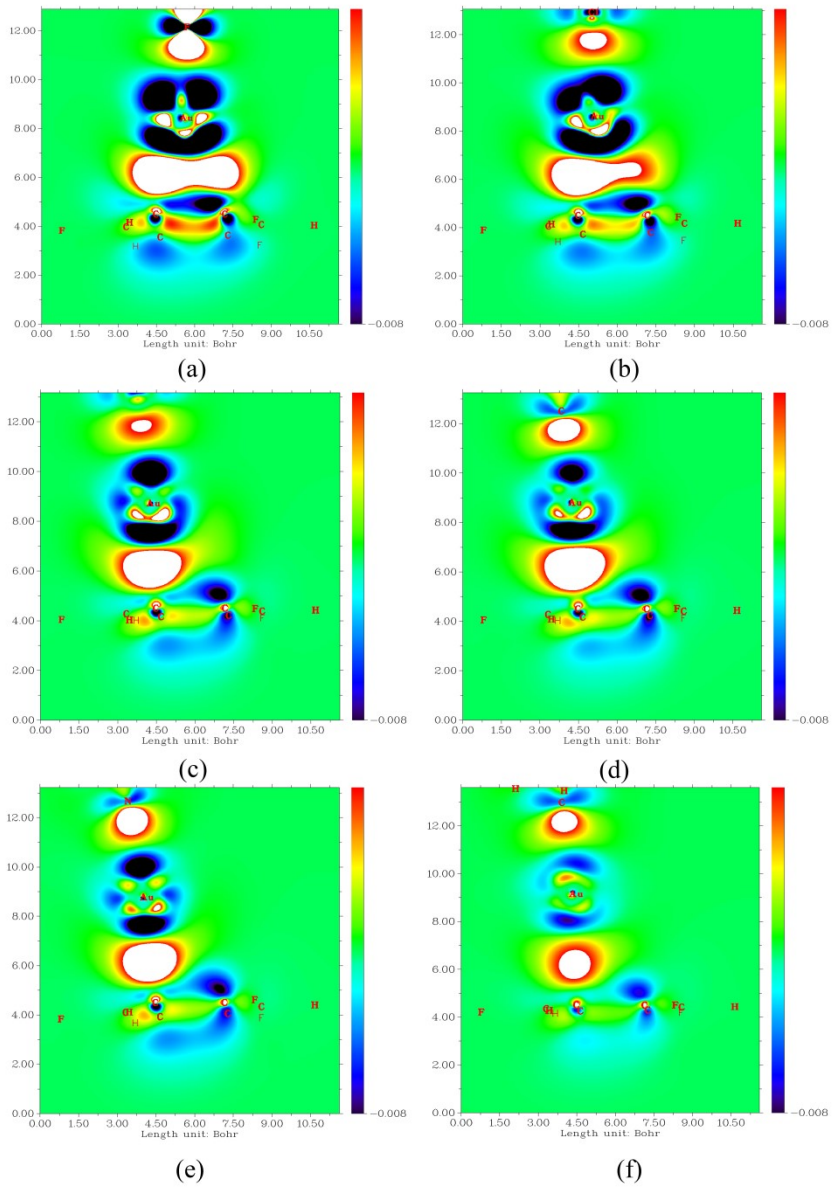


Fig. S5 Computed density difference plots for the complexes TFB···AuX. (a) TFB···AuF, (b) TFB···AuCl, (c) TFB···AuBr, (d) TFB···AuCN, (e) TFB···$AuNO_2$, (f) TFB···$AuCH_3$

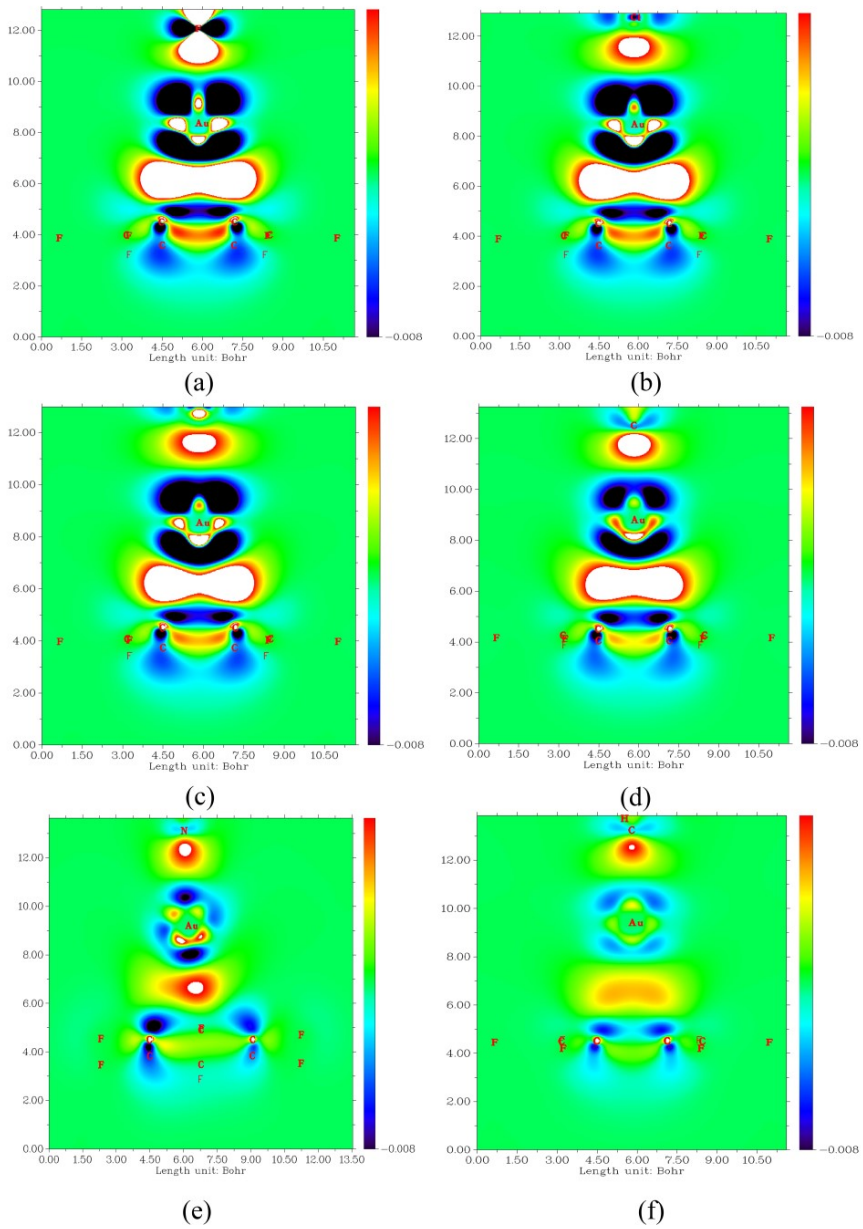


Fig. S6 Computed density difference plots for the complexes HFB···AuX. (a) HFB···AuF; (b) HFB···AuCl; (c) HFB···AuBr; (d) HFB···AuCN; (e) HFB···$AuNO_2$; (f) HFB···$AuCH_3$.