Copper(I) Diselenocarbamate Clusters: Synthesis, Structures and Single-Source Precursors for Cu and Se Composite Materials

Rajendra S. Dhayal, Jian-Hong Liao, Hsing-Nan Hou, Ria Ervilita, Ping-Kuei Liao, and C. W. Liu*

*a Department of Chemistry, National Dong Hwa University, Hualien, Taiwan 97401, R. O. C. E-mail: chenwei@mail.ndhu.edu.tw.

b School of Chemistry and Biochemistry, Thapar University, Patiala 147004, Punjab, India
Figure S1. $^1$H NMR spectra of $[\text{Cu}_8(\text{H})\{\text{Se}_2\text{CN}^n\text{Pr}_2\}_6](\text{PF}_6)$, 2H in CDCl$_3$
Figure S2. $^2$H NMR spectra of $[\text{Cu}_8(\text{D})\{\text{Se}_2\text{CN}^\alpha\text{Pr}_2\}_6](\text{PF}_6)$, $2_\text{D}$ in CH$_2$Cl$_2$
Figure S3. $^1$H NMR spectra [Cu$_8$(H)(Se$_2$CNEt$_2$)$_6$], 3$_H$ in CD$_2$Cl$_2$
Figure S4. $^2$H NMR spectra $[\text{Cu}_8(\text{D})_6\{\text{Se}_2\text{CNEt}_2\}_6]$, $3_D$ in CH$_2$Cl$_2$
Figure S5. $^1$H NMR spectra of [Cu$_7$(H)$\{\text{Se}_2\text{CN}^n\text{Pr}_2\}_6$], $4_H$ in CDCl$_3$
Figure S6. $^2$H NMR spectra of $[\text{Cu}_7(\text{D})\{\text{Se}_2\text{CN}^n\text{Pr}_2\}_6]$, $4_\text{D}$ in CHCl$_3$.

Figure S7. $^1$H NMR spectra of $[\text{Cu}_7(\text{H})\{\text{Se}_2\text{CNEt}_2\}_6]$, $5_\text{H}$ in CD$_2$Cl$_2$.

Figure S8. $^2$H NMR spectra of $[\text{Cu}_7(\text{D})\{\text{Se}_2\text{CNEt}_2\}_6]$, $5_\text{D}$ in THF.
Figure S9. $^{77}\text{Se}$ NMR spectra of $[\text{Cu}_8(\text{H})\{\text{Se}_2\text{CN}^\mu\text{Pr}_2\}_6](\text{PF}_6)$, $2_\text{H}$ in CHCl$_3$. 
Figure S10. $^{77}\text{Se}$ NMR spectra of $[\text{Cu}_8(\text{H})\{\text{Se}_2\text{CNEt}_2\}_6]\text{PF}_6$, $3_H$ in CH$_2$Cl$_2$

Figure S11. $^{77}\text{Se}$ NMR spectra $[\text{Cu}_7(\text{H})\{\text{Se}_2\text{CN}^\text{Bu}_2\}_6]$, $4_H$ in CHCl$_3$
Figure S12. $^{77}\text{Se}$ NMR spectra of [Cu$_7$(H){Se$_2$CNEt$_2$}$_6$], 5$_\text{II}$ in CH$_2$Cl$_2$
Figure S13. ESI-MS spectrum of $[\text{Cu}_8(\text{H})\{\text{Se}_2\text{CNPr}_2\}_6]^+$, $2_\text{H}$. The inset shows experimental (a) and theoretical one (b).
Figure S14. ESI-MS spectrum of $[\text{Cu}_8(\text{H})\{\text{Se}_2\text{CNEt}_2\}_6]^+$, $3_H$. The inset shows experimental (a) and theoretical one (b).
Figure S15. ESI-MS spectrum of $[\text{Cu}_7(\text{H})\{\text{Se}_2\text{CN}^\text{Pr}_2\}_6]^+$, $4_\text{II}$, observed an adduct species $[\text{Cu}_7(\text{H})\{\text{Se}_2\text{CN}^\text{Pr}_2\}_6(\text{Cu})]^+$, $[4_\text{II} + \text{Cu}]^+$. 
Figure S16. ESI-MS spectrum of [Cu$_7$(H)$_6$(Se$_2$CNEt$_2$)$_6$], $5_H$, observed an adduct species [Cu$_7$(H)$_6$(Se$_2$CNEt$_2$)$_6$(Cu)]$^+$, $[5_H + Cu]^+$. 