Hexafluorosilicate anion in formation of coordination cage: anion competition

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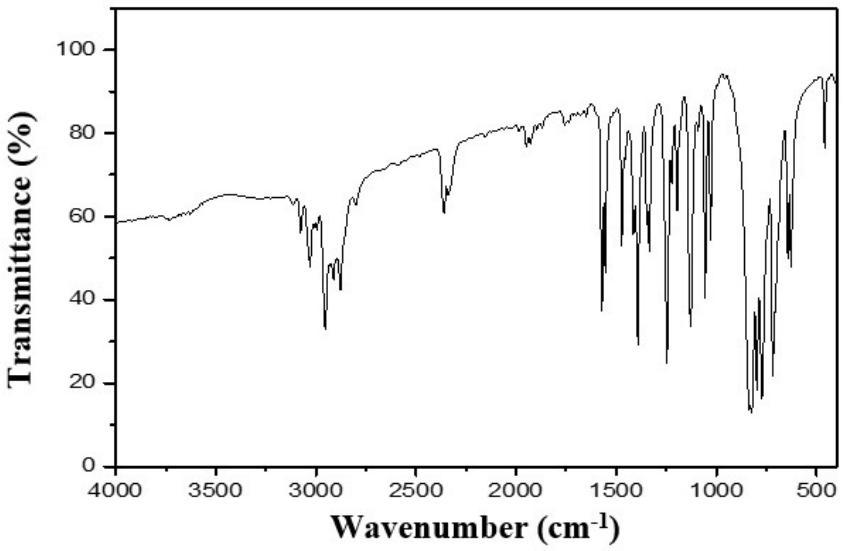
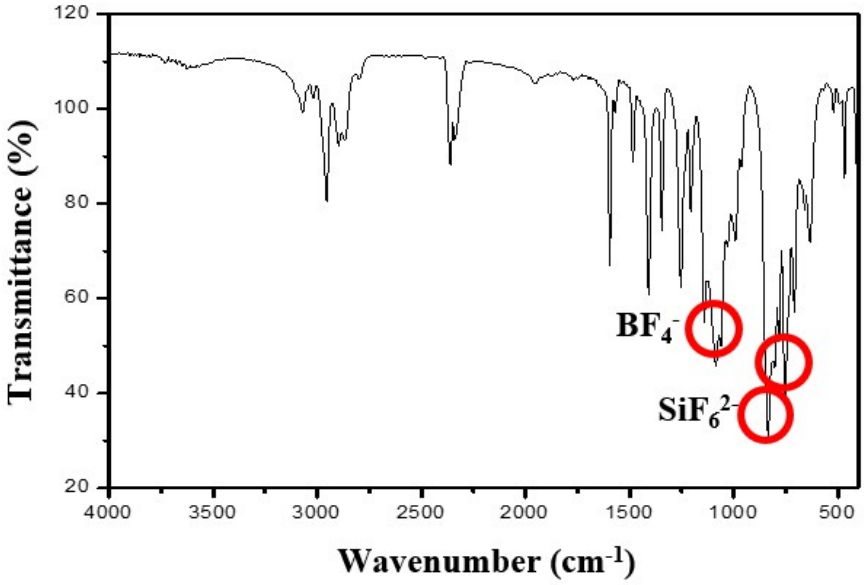
Electronic supplementary information (ESI) available: IR spectra and TGA-DSC curves of $[(SiF_6)@Cu_2L_4](BF_4)_2\cdot MeOH$, $[(SiF_6)@Cu_2L_4](SiF_6)\cdot 6MeOH$ and $[Cu(PF_6)_2L_2]\cdot C_3H_6O$; crystallographic data of $[(SiF_6)@Cu_2L_4](BF_4)_2\cdot MeOH$, $[(SiF_6)@Cu_2L_4](SiF_6)\cdot 6MeOH$ and $[Cu(PF_6)_2L_2]\cdot C_3H_6O$; UV spectra of $[(SiF_6)@Cu_2L_4](BF_4)_2\cdot MeOH$, $[(SiF_6)@Cu_2L_4](SiF_6)\cdot 6MeOH$, $[Cu(PF_6)_2L_2]\cdot C_3H_6O$ and $Cu(BF_4)_2$; ESI-TOF-MS of $[(SiF_6)@Cu_2L_4](BF_4)_2\cdot MeOH$; ^{13}C NMR spectra of 1,2-bis(dimethyl(pyridin-3-yl)silyl)ethane. CCDC 1955858, 1955860, 1955861. For ESI and crystallographic data in CIF or other electronic format see DOI:

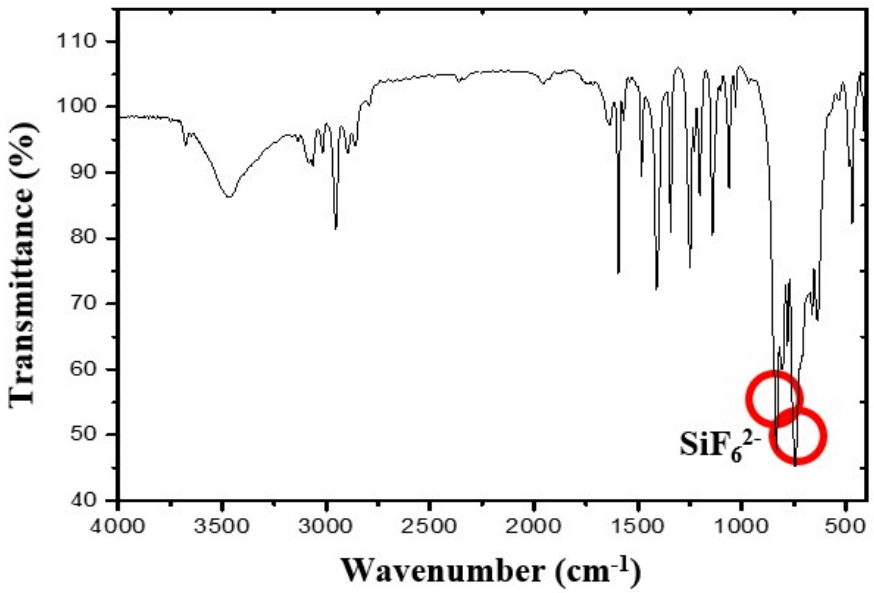
1,2-bis(dimethyl(pyridin-3-yl)silyl)ethane (L)



$[(SiF_6)@Cu_2L_4](BF_4)_2 \cdot MeOH$



[(SiF$_6$)@Cu$_2$L$_4$](SiF$_6$)·6MeOH



[Cu(PF$_6$)$_2$L$_2$]· C$_3$H$_6$O

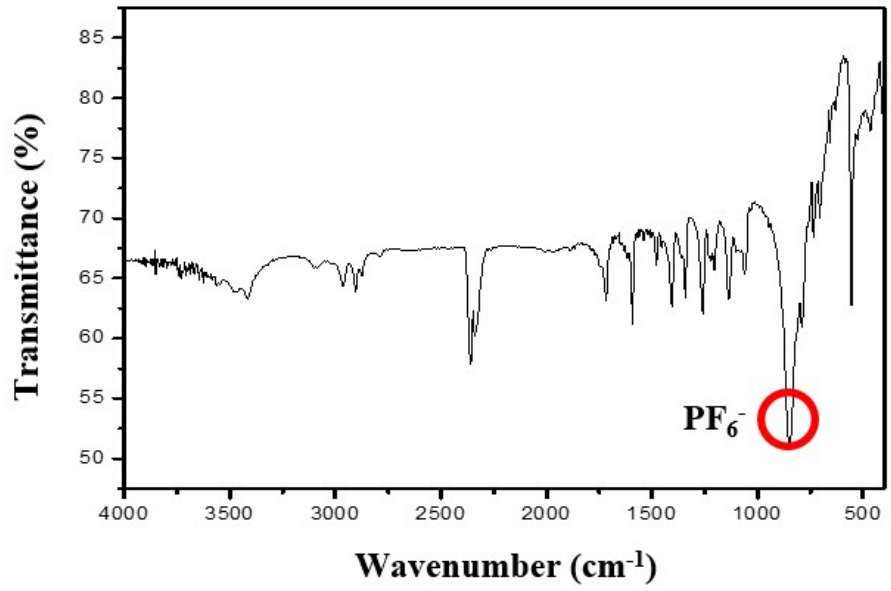
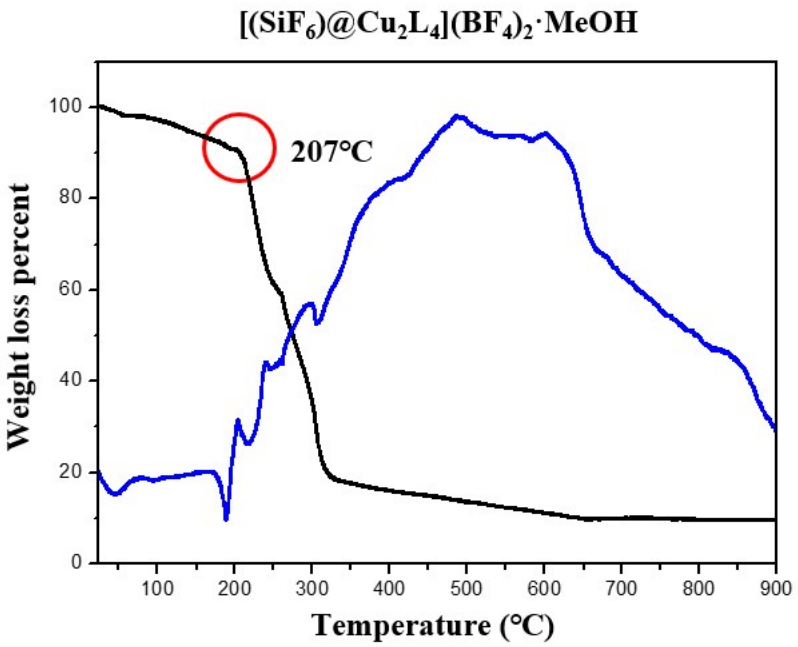
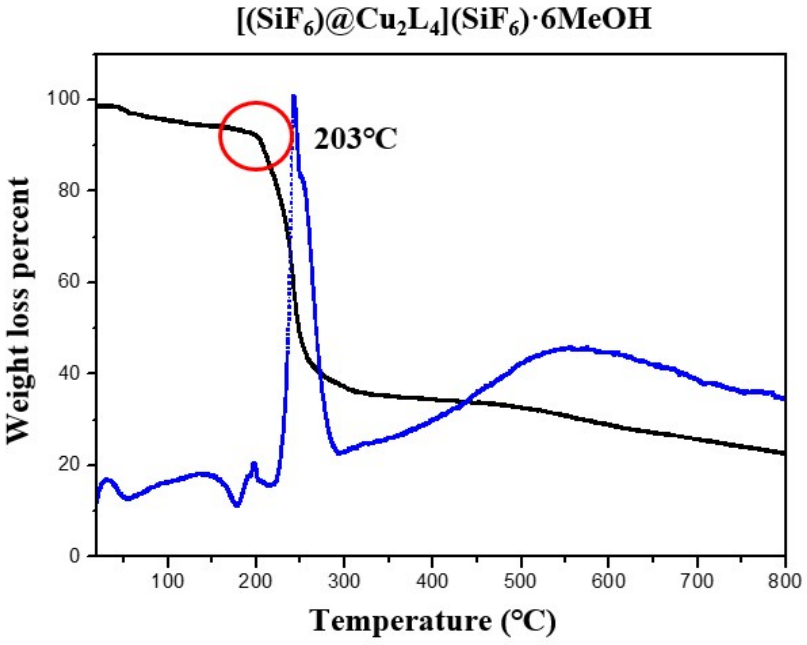


Fig. S1 IR spectra of 1,2-bis(dimethyl(pyridin-3-yl)silyl)ethane (L), [(SiF$_6$)@Cu$_2$L$_4$](BF$_4$)$_2$·MeOH, [(SiF$_6$)@Cu$_2$L$_4$](SiF$_6$)·6MeOH and [Cu(PF$_6$)$_2$L$_2$]· C$_3$H$_6$O


[(SiF6)@Cu2L4](BF4)2·MeOH
207°C
Weight loss percent
Temperature (°C)
0
20
40
60
80
100
100
200
300
400
500
600
700
800
900


[(SiF6)@Cu2L4](SiF6)·6MeOH
203°C
Weight loss percent
Temperature (°C)
0
20
40
60
80
100
100
200
300
400
500
600
700
800

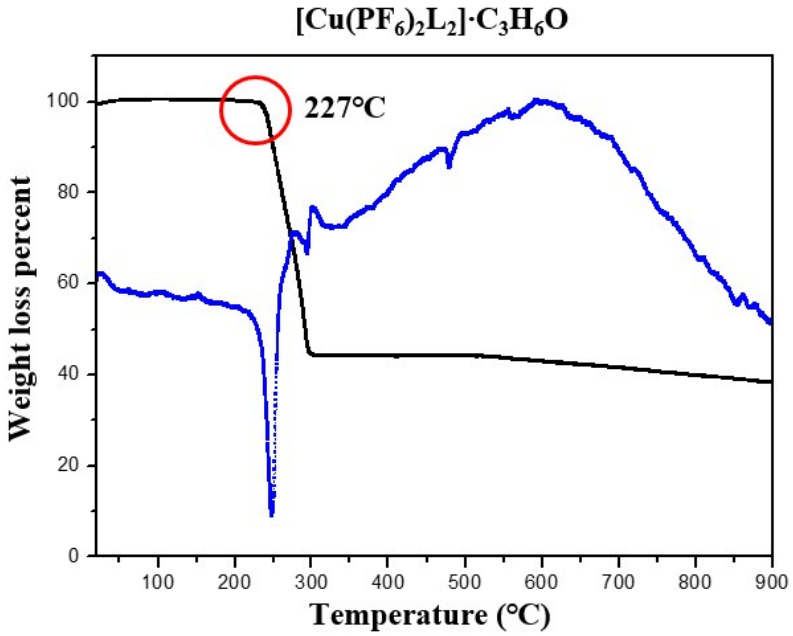
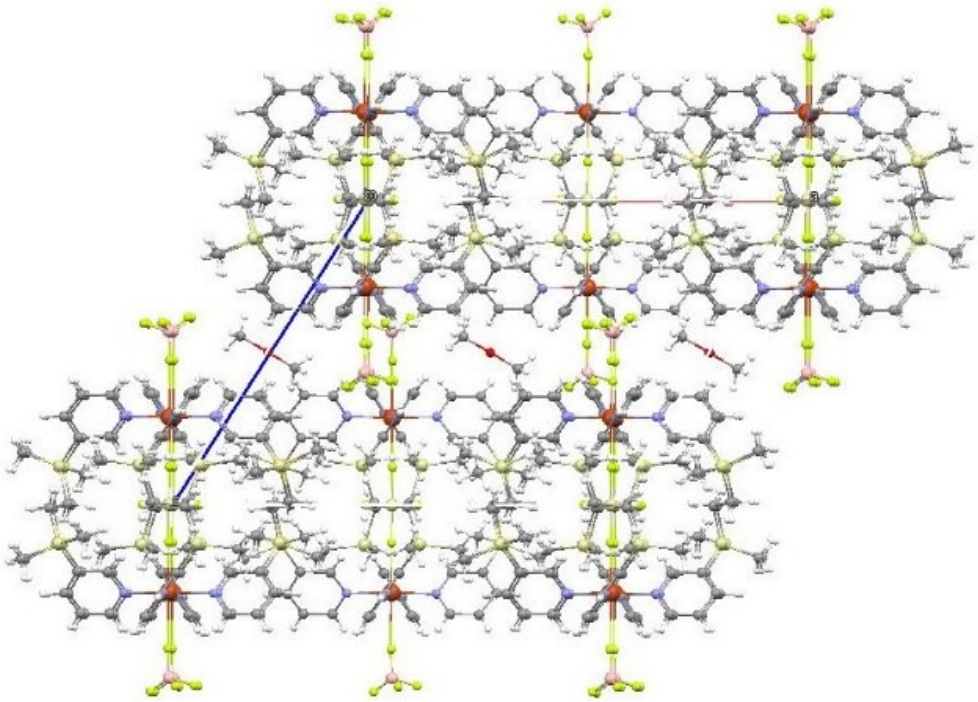
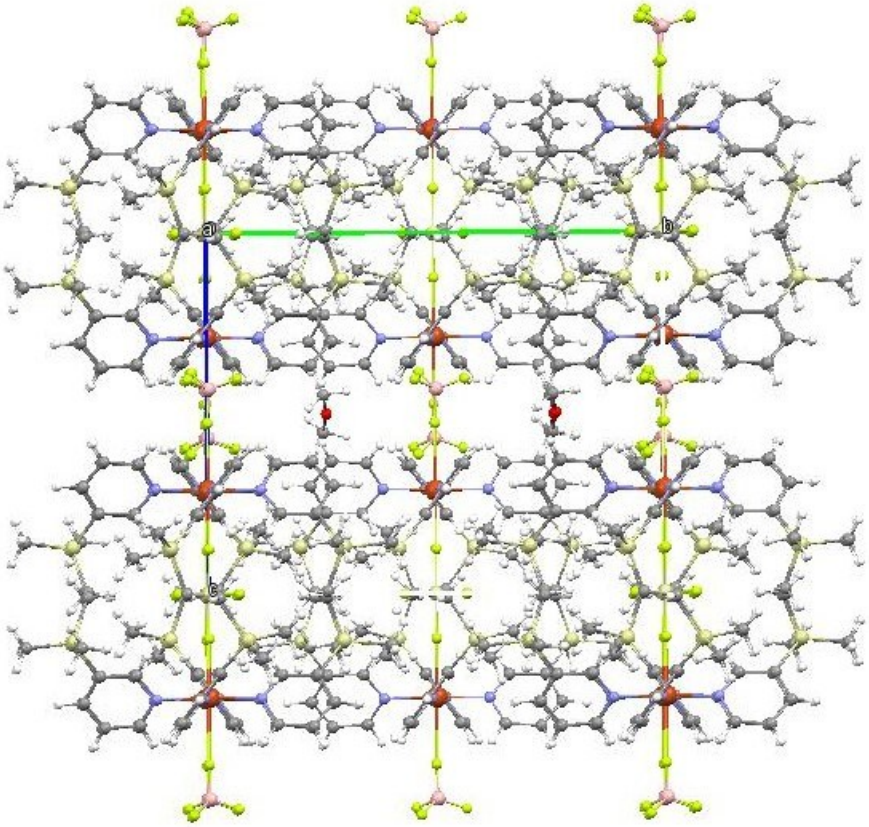
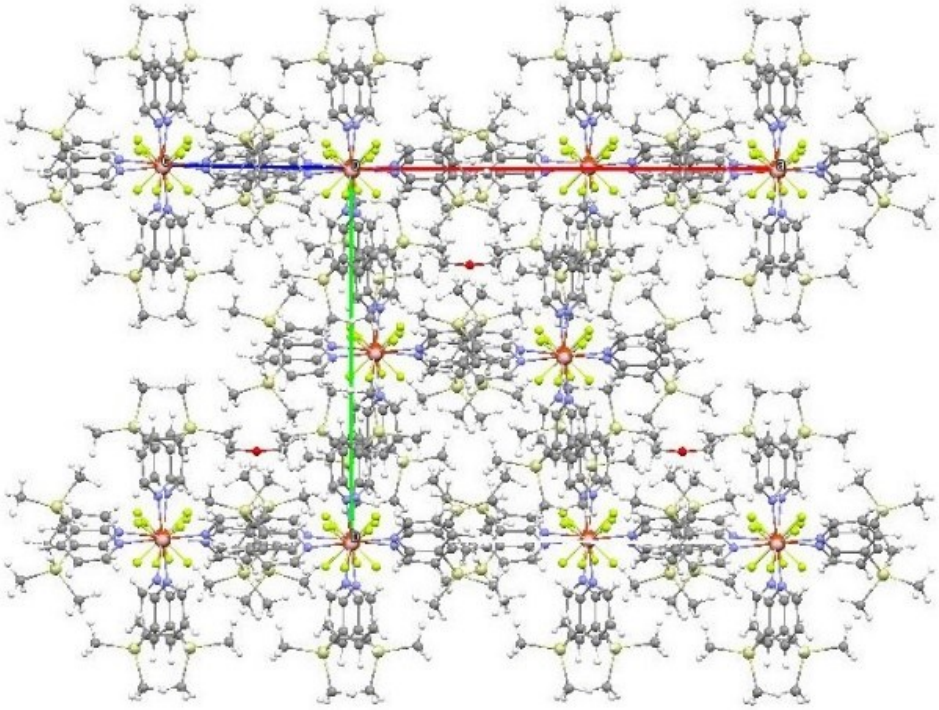


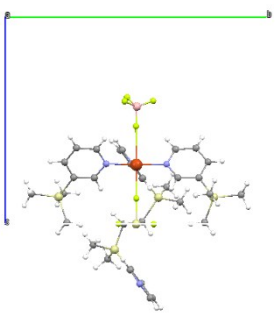
Fig. S2 TG and DSC curves of $[(SiF_6)@Cu_2L_4](BF_4)_2 \cdot MeOH$, $[(SiF_6)@Cu_2L_4](SiF_6) \cdot 6MeOH$ and $[Cu(PF_6)_2L_2] \cdot C_3H_6O$

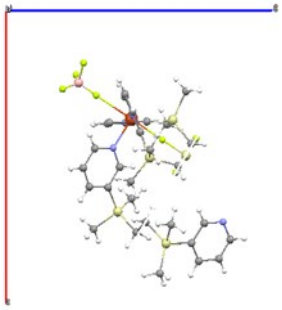
$[(SiF_6)@Cu_2L_4](BF_4)_2 \cdot MeOH$

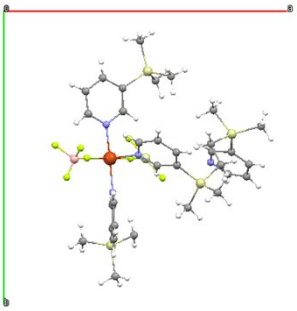




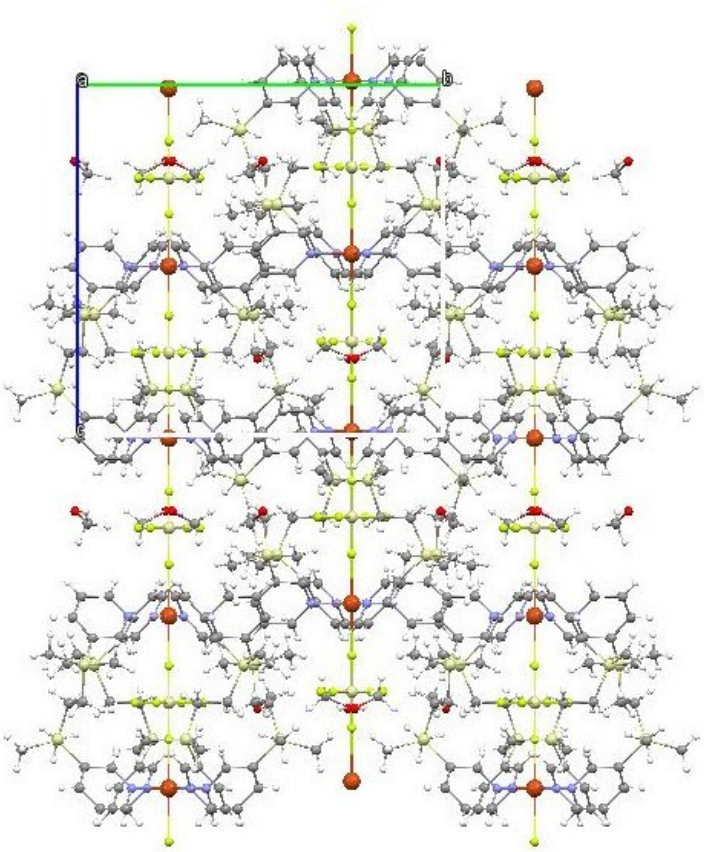


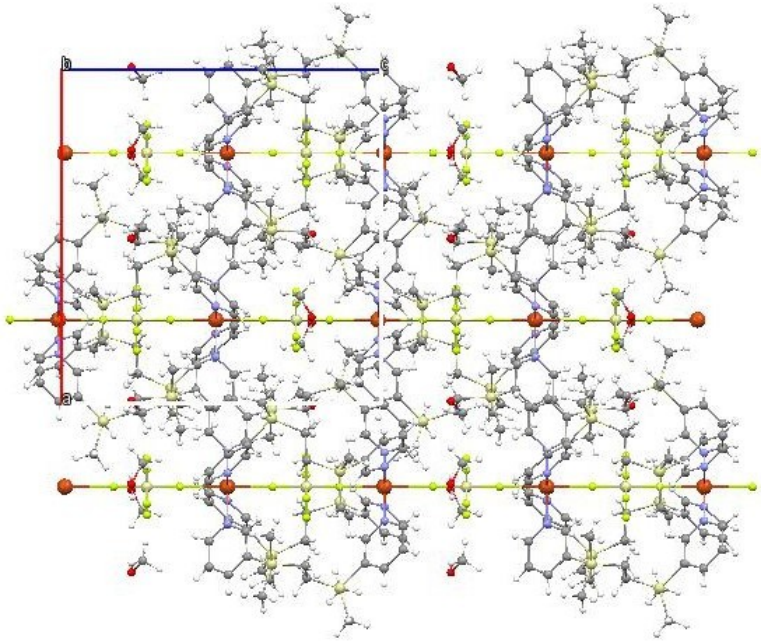


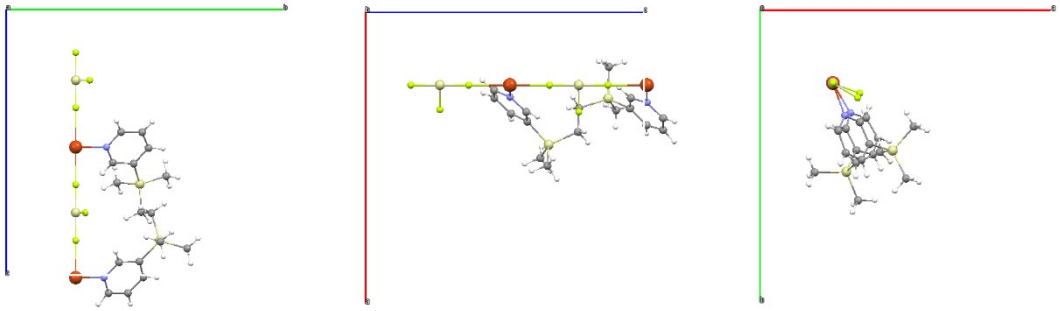


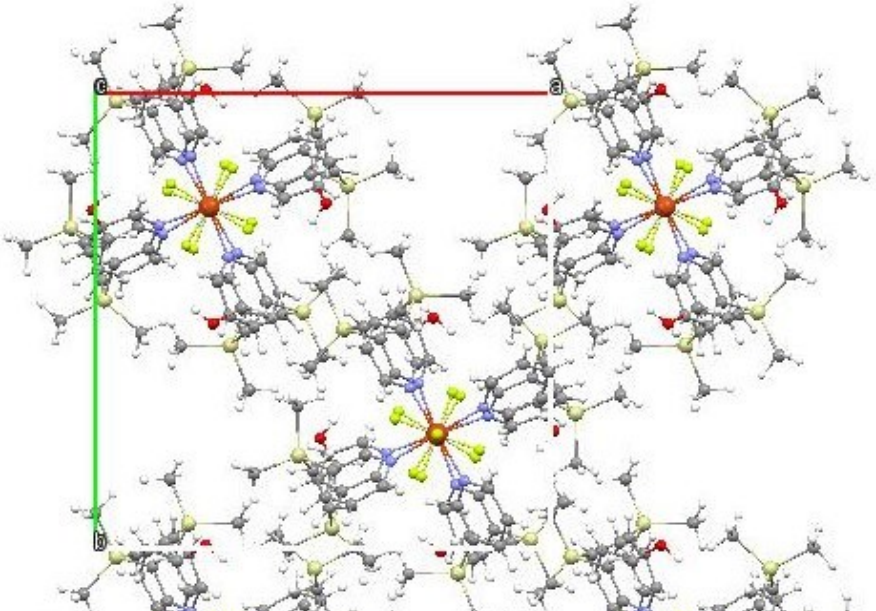


[(SiF_6)@Cu_2L_4](SiF_6)·6MeOH

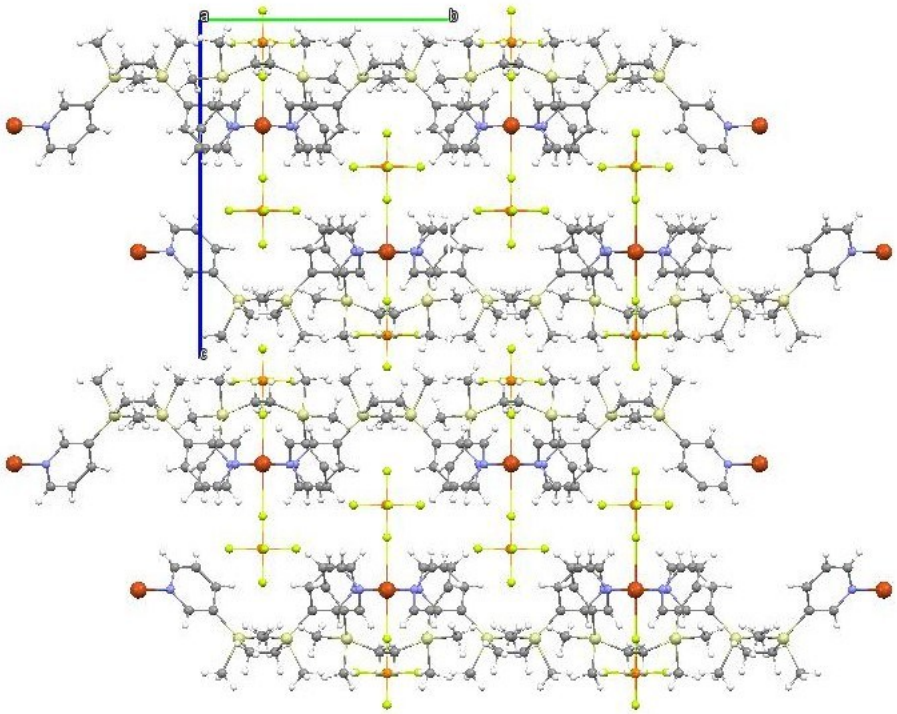


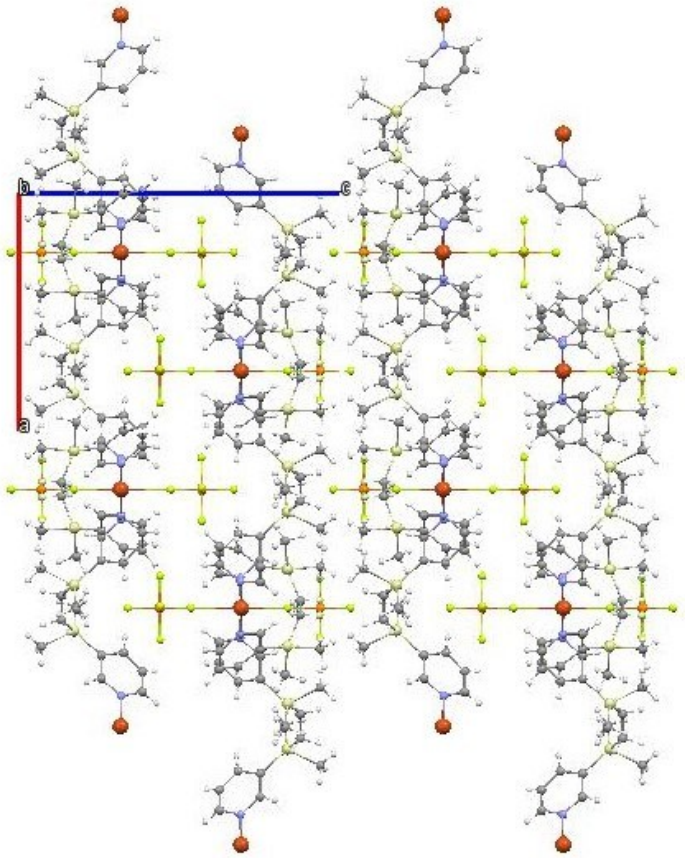





c
a
b

$[Cu(PF_6)_2L_2]\cdot C_3H_6O$





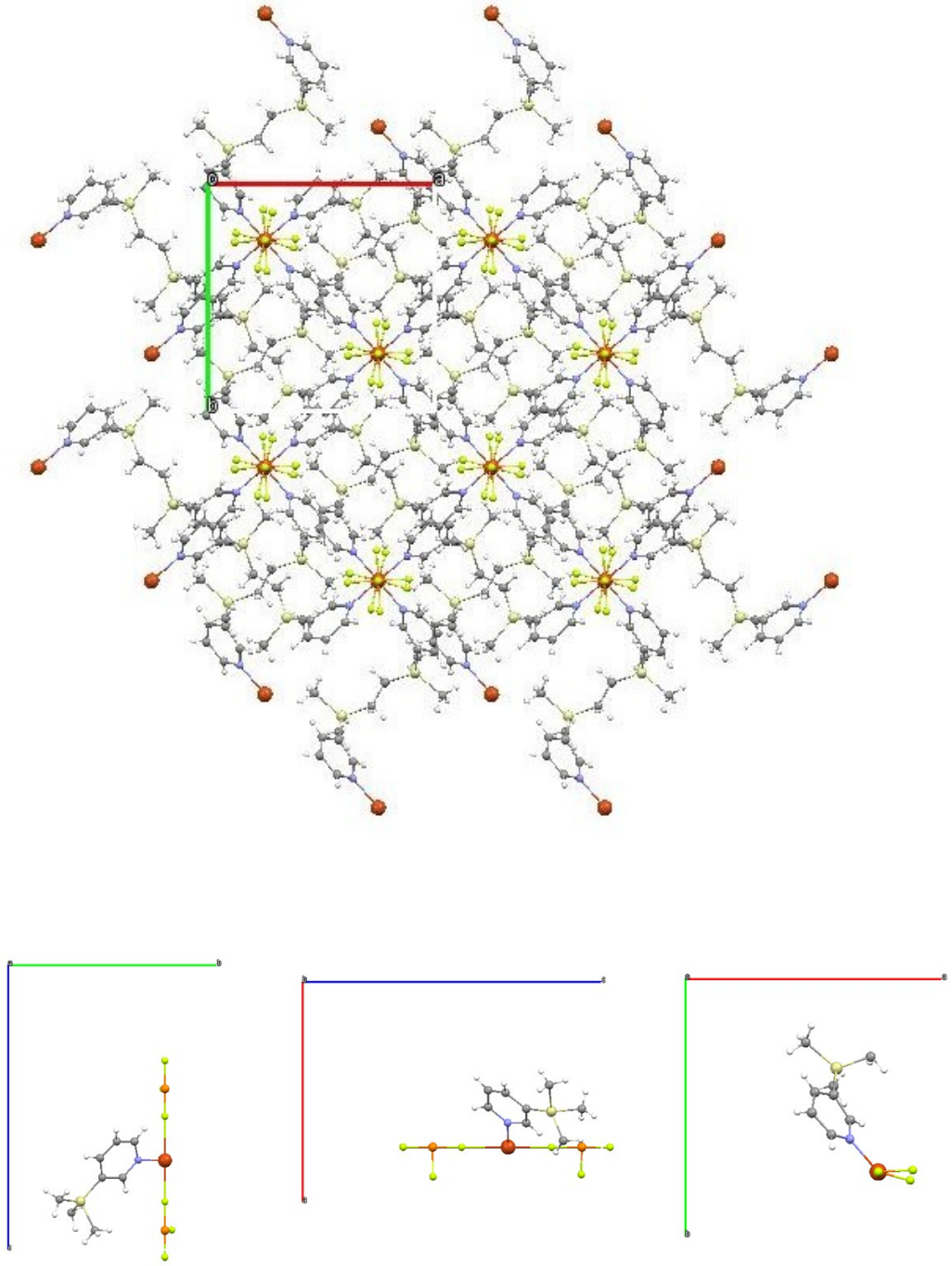
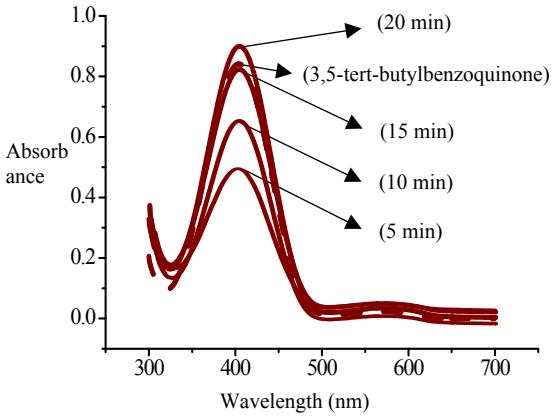
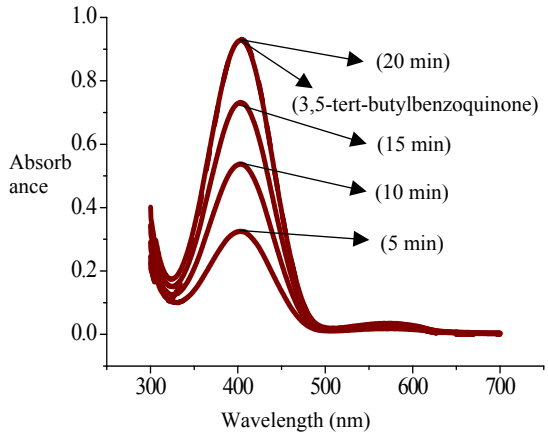


Fig. S3 Packing structures and asymmetric units of $[(SiF_6)@Cu_2L_4](BF_4)_2 \cdot MeOH$, $[(SiF_6)@Cu_2L_4](SiF_6) \cdot 6MeOH$ and $[Cu(PF_6)_2L_2] \cdot C_3H_6O$.

[(SiF$_6$)@Cu$_2$L$_4$](BF$_4$)$_2$·MeOH



[(SiF$_6$)@Cu$_2$L$_4$](SiF$_6$)·6MeOH



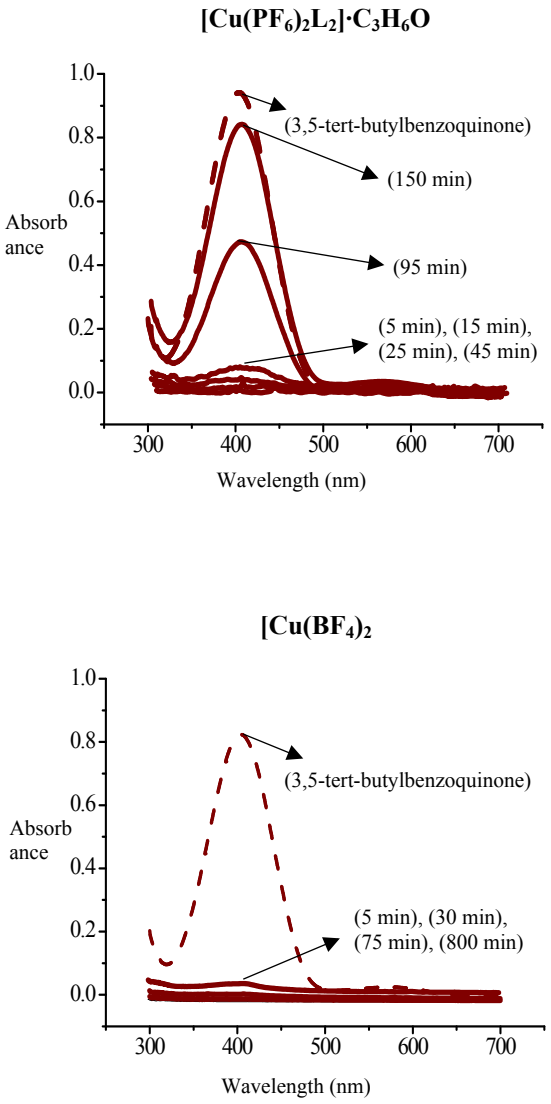


Fig. S4 UV spectral change on the catechol oxidation catalysis using the following catalyst.

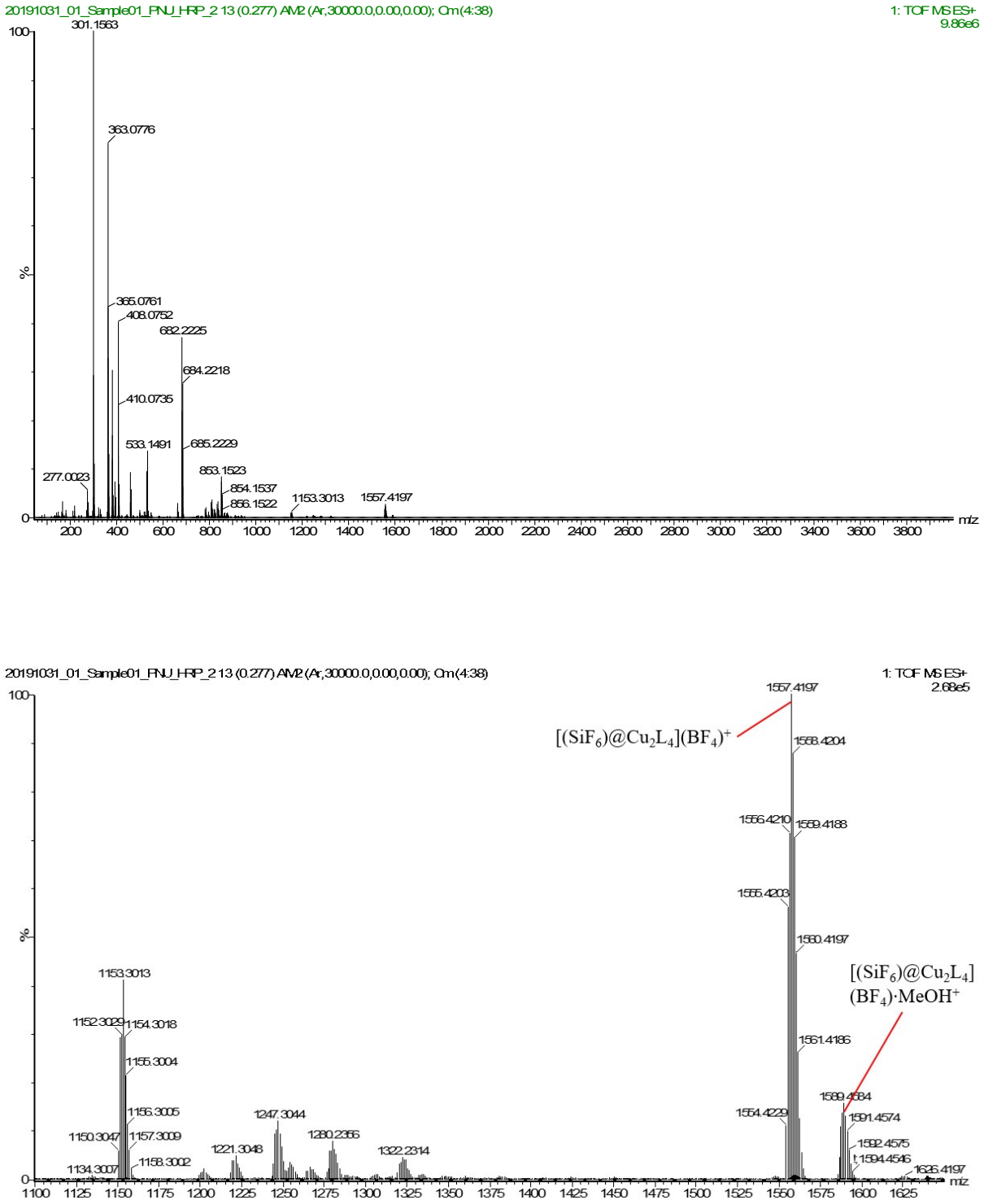


Fig. S5 Electrospray time of flight ionization mass spectrometry (ESI-TOF-MS) data of $[(SiF_6)@Cu_2L_4](BF_4)_2 \cdot MeOH$. m/z range 0-4000 (top), m/e range 1100-1650 (bottom). m/z for $[(SiF_6)@Cu_2L_4](BF_4) \cdot MeOH^+$ = 1589.46; m/z for $[(SiF_6)@Cu_2L_4](BF_4)^+$ = 1557.41

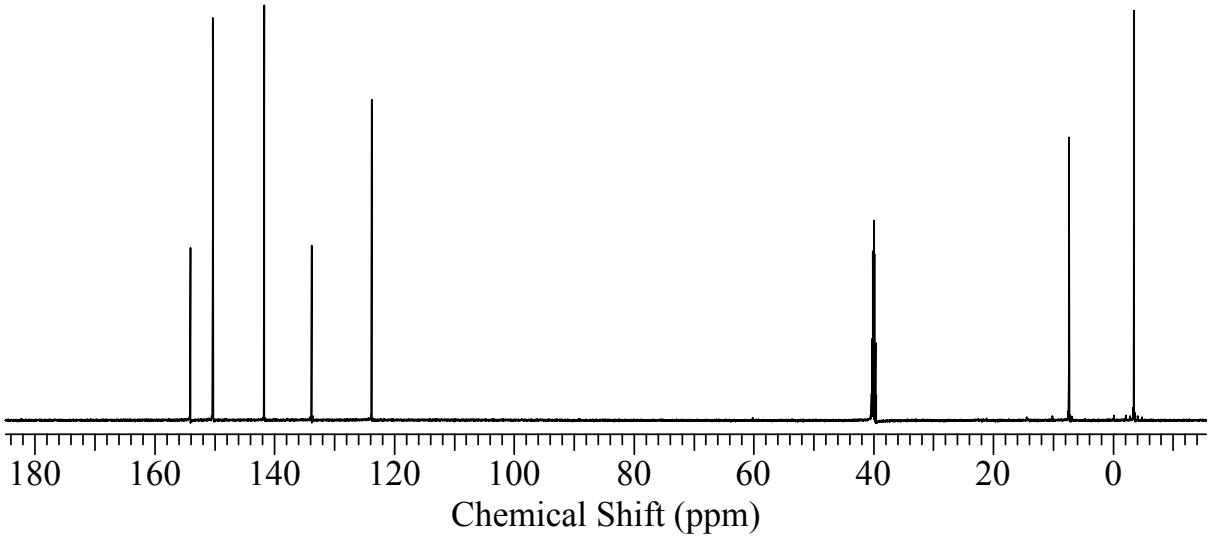


Fig. S6 ^{13}C NMR spectra of 1,2-bis(dimethyl(pyridin-3-yl)silyl)ethane (L)