

Fig. S1 Optical absorption spectra of species **2** in CH_2Cl_2 generated at (A) 193K, (B) 243 (C) 263 K (solid line). The spectra fitting (dotted line) was performed with Fit Multi-peaks Gaussian model by using the Origin 6.0 Professional Microcal Software.

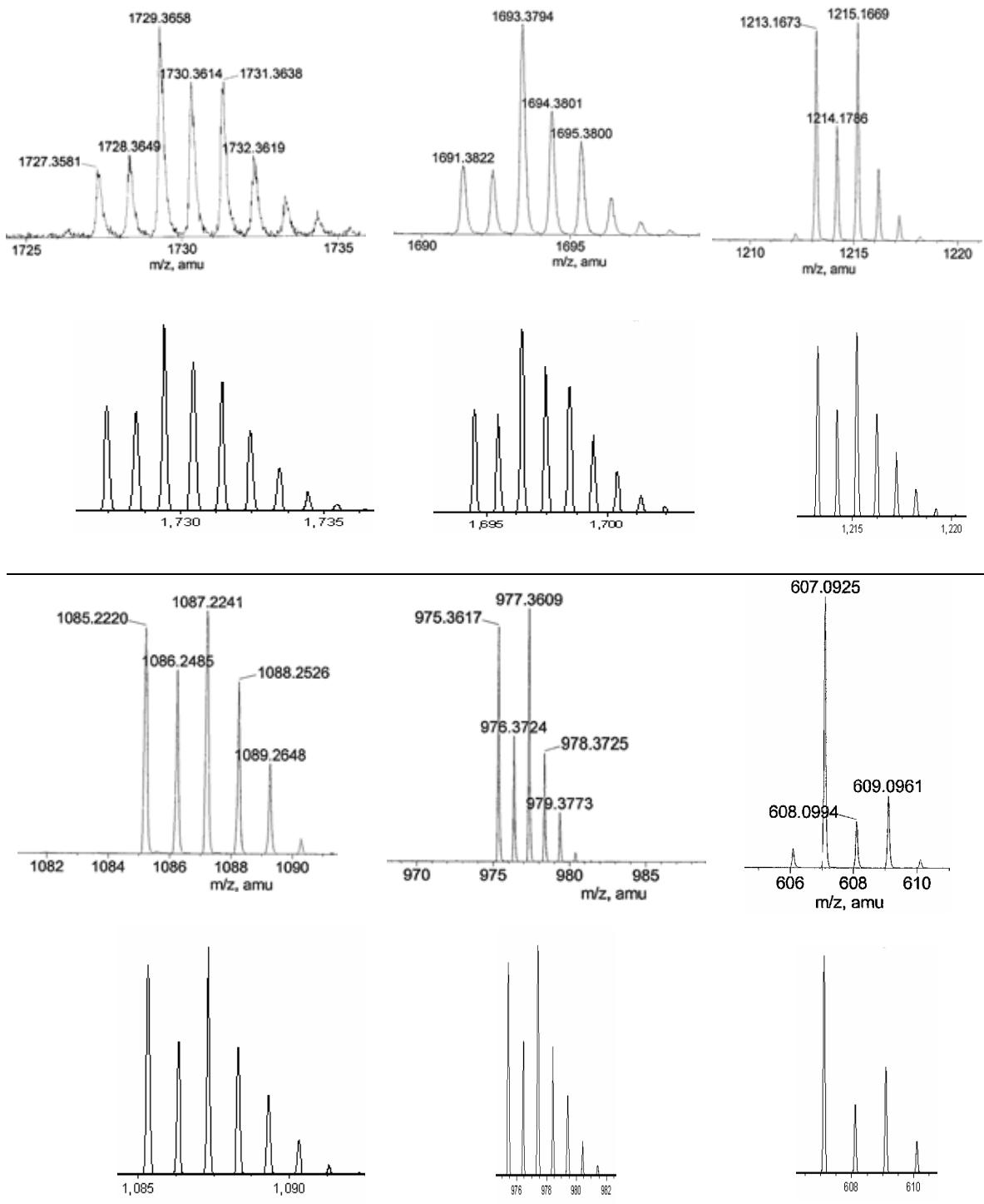


Fig. S2 Sections of TOF-MS (top) and simulation (bottom) for the oxygenated species **2** showing the observed and calculated distribution isotope patterns for positive ion clusters.

Table S-1. Selected bond distances (\AA) and angles ($^\circ$) for $[\text{Cu}(\text{L})\text{Cl}]\text{Cl}\cdot 2\text{CHCl}_3$ (**4** \cdot 2CHCl_3).

Cu–Cl(1)	2.2441(7)	Cu–N(2)	1.983(2)
Cu–N(1)	2.0364(19)	Cu–N(3)	1.982(2)
Cu–O(1)	2.460(5)	Cu–Cl(18)	4.524
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N(3)–Cu–N(2)	165.06(9)	N(3)–Cu–Cl(1)	96.47(6)
N(3)–Cu–N(1)	82.08(8)	N(2)–Cu–Cl(1)	97.36(6)
N(2)–Cu–N(1)	83.70(8)	N(1)–Cu–Cl(1)	175.52(6)