

Electronic Supplementary Information

Assembly of bicyclic or monocyclic clusters from $[(\eta^5\text{-C}_5\text{Me}_5)_2\text{Mo}_2(\mu_3\text{-S})_4(\text{CuMeCN})_2]^{2+}$ with tetrphosphine or N,P mixed ligands: syntheses, structures and enhanced third-order NLO performances

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10

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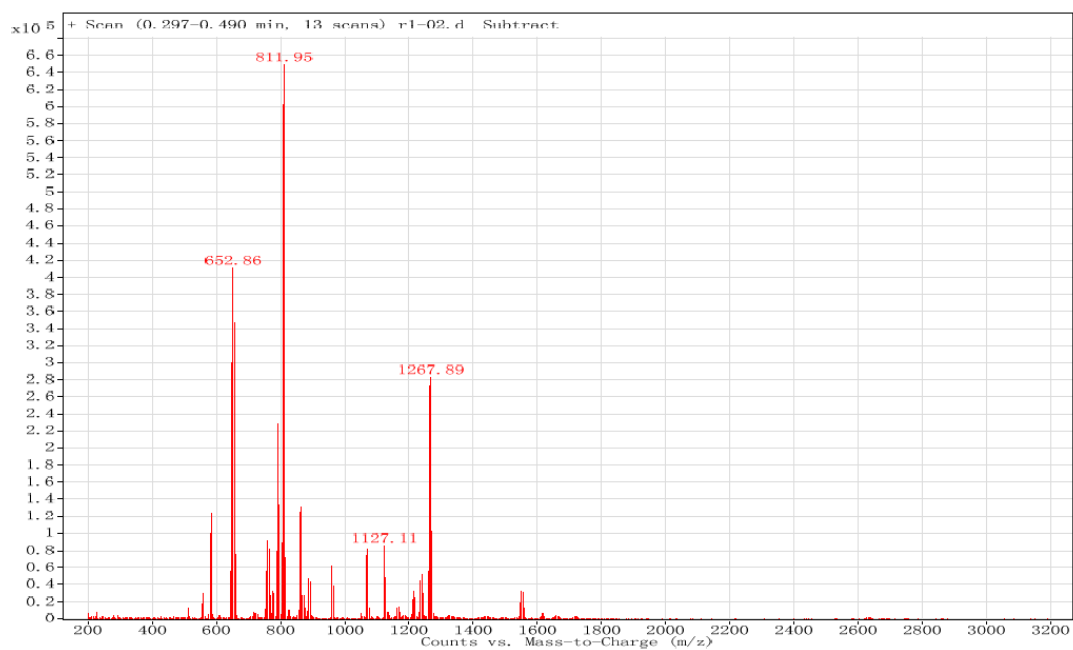
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Figure S1. ESI MS data of **3**. (a) The full data ranging from $m/z = 200-3200$; (b) tested (black) and simulated (gray) data at $m/z = 811.9$; (c) tested (black) and simulated (gray) data at $m/z = 584.0$ S3

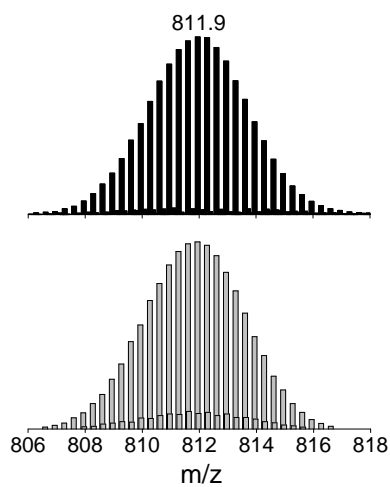
Figure S2. The full data ESI MS data of **4** (a), **5** (b) and **6** (c) ranging from $m/z = 200-3200$ in MeCN.S4

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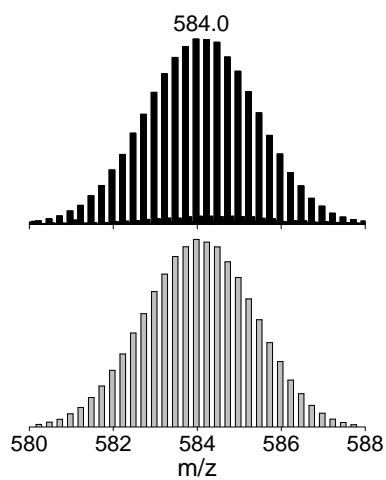
Figure S3. The DFWM signal of a 1×10^{-4} M MeCN solution for **1** (a), **4** (b), **5** (c) and **6** (d) with 50-fs laser and 1.5 mm cell. The black squares are experimental data, and the solid curve is the theoretical fit.S5



(a)

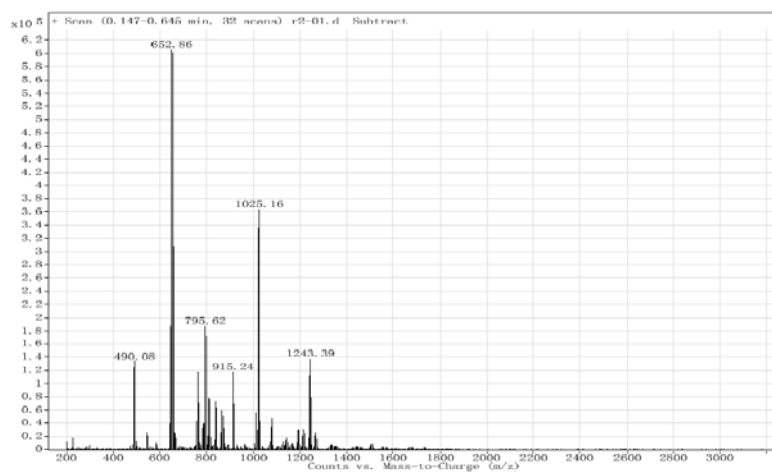


(b)

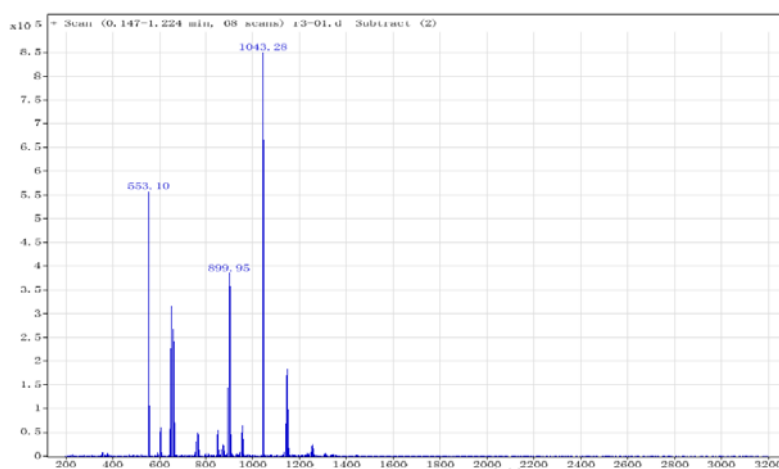


(c)

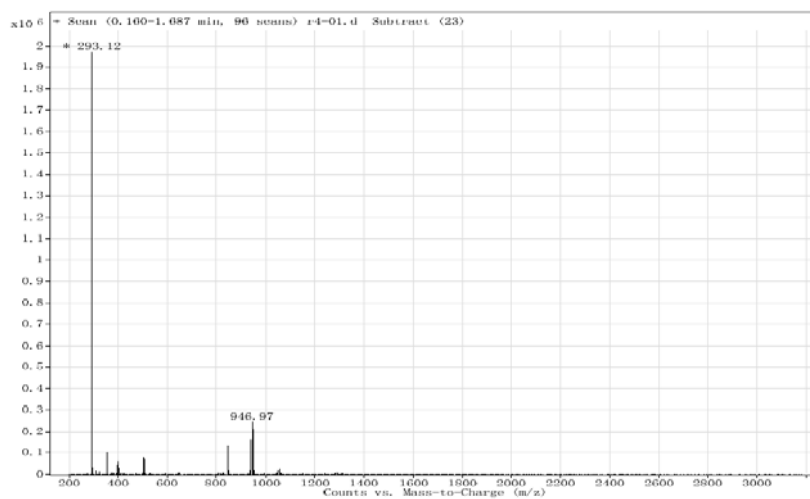
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Figure S1. ESI MS data of **3** in MeCN. (a) The full data ranging from $m/z = 200$ - 3200 ; (b) tested (black) and simulated (gray) data at $m/z = 811.9$; (c) tested (black) and simulated (gray) data at $m/z = 584.0$



(a)

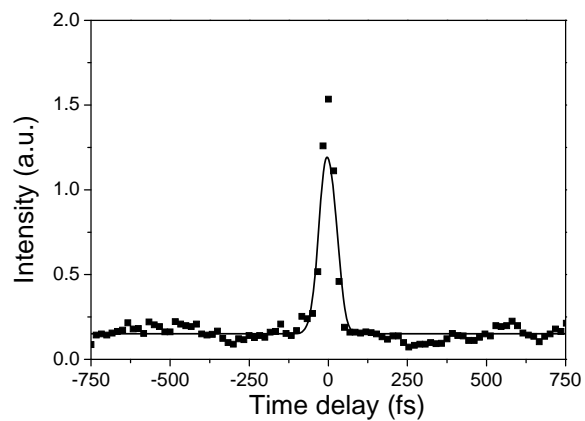


(b)

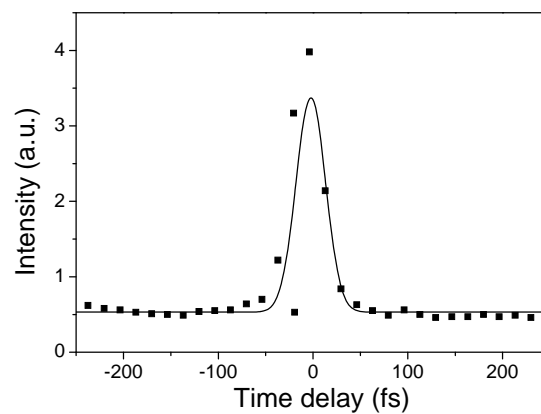


(c)

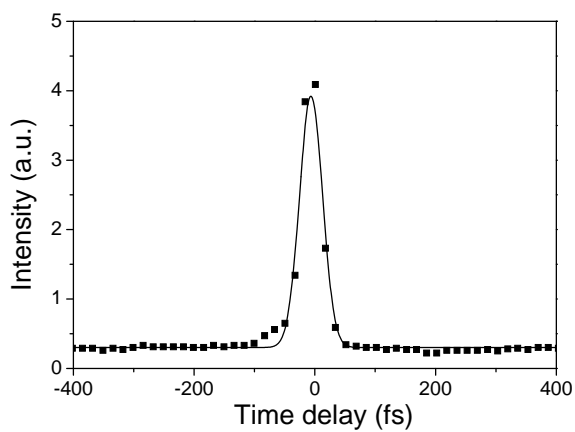
Figure S2. The full data ESI MS data of **4** (a), **5** (b) and **6** (c) ranging from $m/z = 200-3200$ in MeCN.



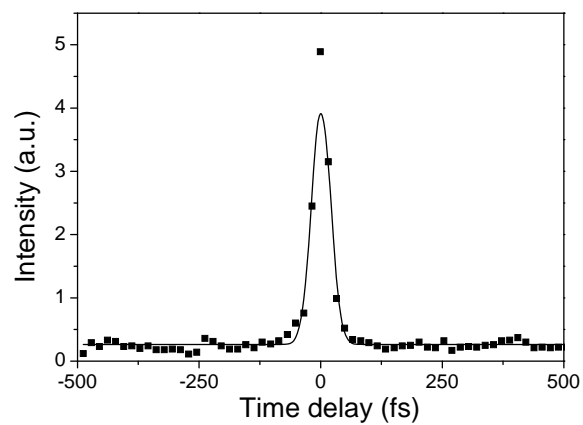
(a)



(b)



(c)



(d)

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Figure S3 The DFWM signal of a 1×10^{-4} M MeCN solution for **1** (a), **4** (b), **5** (c) and **6** (d) with 50-fs laser and 1.5 mm cell. The black squares are experimental data, and the solid curve is the theoretical fit.