Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Electronic Supplementary Informations

For

Syntheses, crystal structures, magnetochemistry and catechol oxidase activity of a tetracopper(II) compound and a new type of dicopper(II)-based 1D coordination polymer

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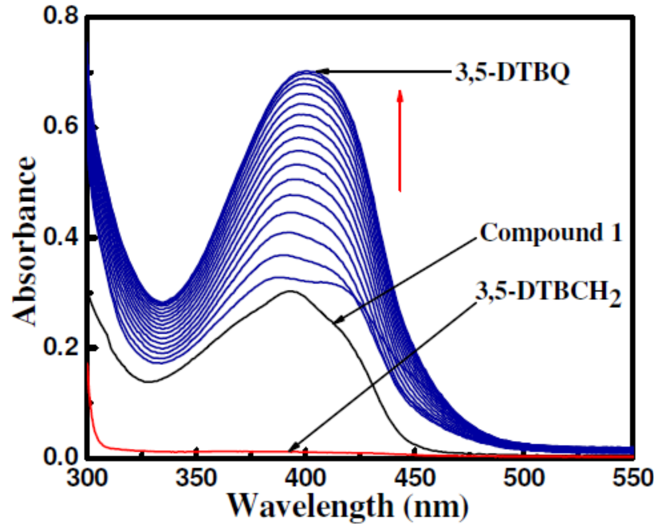

Fig. S1 The spectral profile showing the increase of quinone band at 400 nm after the addition of 100 fold of 3,5-DTBCH$_2$ to a solution containing complex [$Cu_4L_2(\mu_3$-$OH)_2(NCO)_4$].2H_2O (**1**) (0.25×10^{-4} M) in DMF. The spectra were recorded after every 5 min.

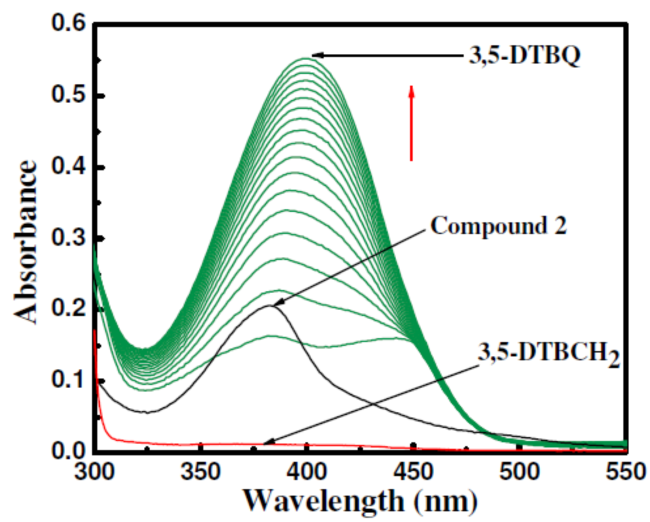

Fig. S2 The spectral profile showing the increase of quinone band at 400 nm after the addition of 100 fold of 3,5-DTBCH$_2$ to a solution containing complex [{{$Cu^{II}_2L(\mu_{1,1}$-$N_3)$}$_2(\mu_{1,1}$-$N_3)_2$}$(\mu_{1,3}$-$N_3)_2]_n$ (**2**) (0.25×10^{-4} M) in acetonitrile. The spectra were recorded after every 5 min.

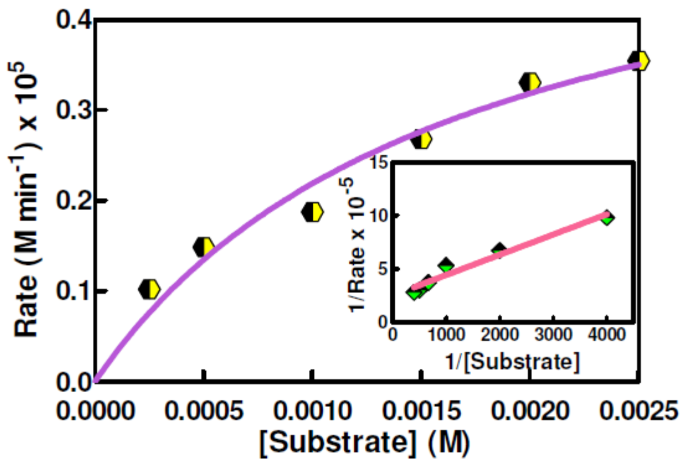

Fig. S3 Initial rates versus substrate concentration for the 3,5-DTBCH_2→3,5-DTBQ oxidation reaction catalyzed by complex $[Cu_4L_2(\mu_3\text{-}OH)_2(NCO)_4].2H_2O$ (**1**) in DMF. Inset shows Lineweaver-Burk plot. Symbols and solid lines represent the observed and simulated profiles, respectively.

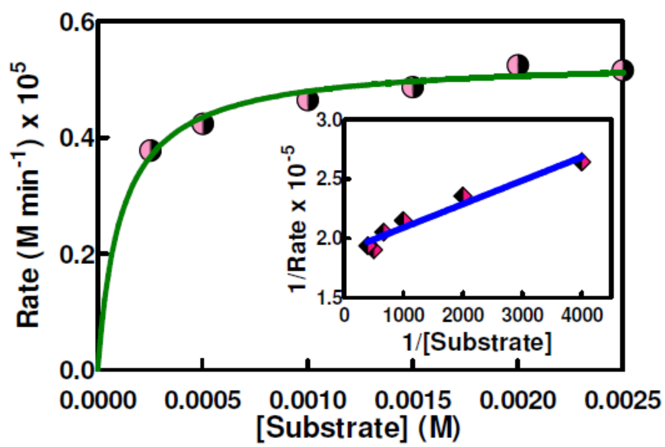

Fig. S4 Initial rates versus substrate concentration for the 3,5-DTBCH_2→3,5-DTBQ oxidation reaction catalyzed by complex $[\{\{Cu^{II}_2L(\mu_{1,1}\text{-}N_3)\}_2(\mu_{1,1}\text{-}N_3)_2\}(\mu_{1,3}\text{-}N_3)_2]_n$ (**2**) in acetonitrile. Inset shows Lineweaver-Burk plot. Symbols and solid lines represent the observed and simulated profiles, respectively.

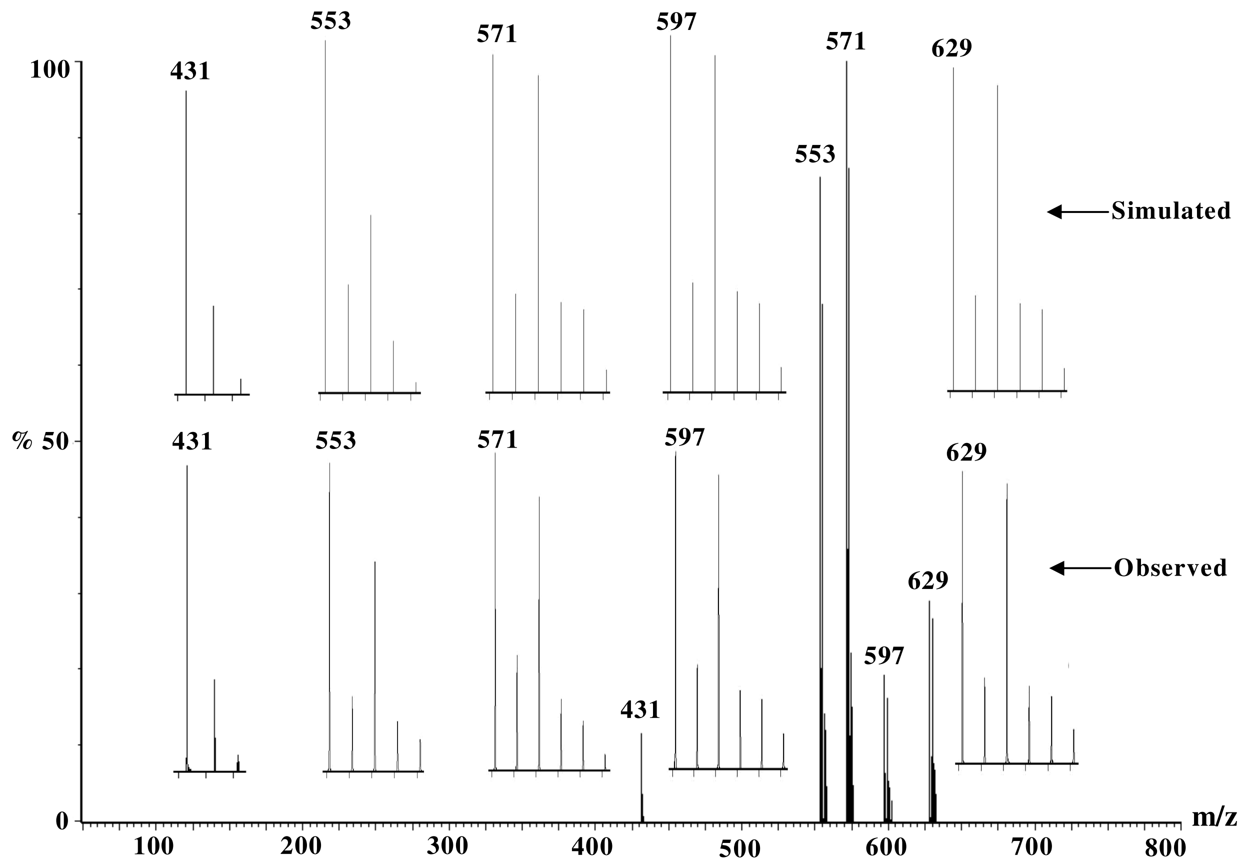

Fig. S5 Electrospray ionization mass spectrum (ESI-MS positive) of $[Cu_4L_2(\mu_3\text{-}OH)_2(NCO)_4].2H_2O$ (**1**) in acetonitrile showing observed and simulated isotopic distribution patterns.

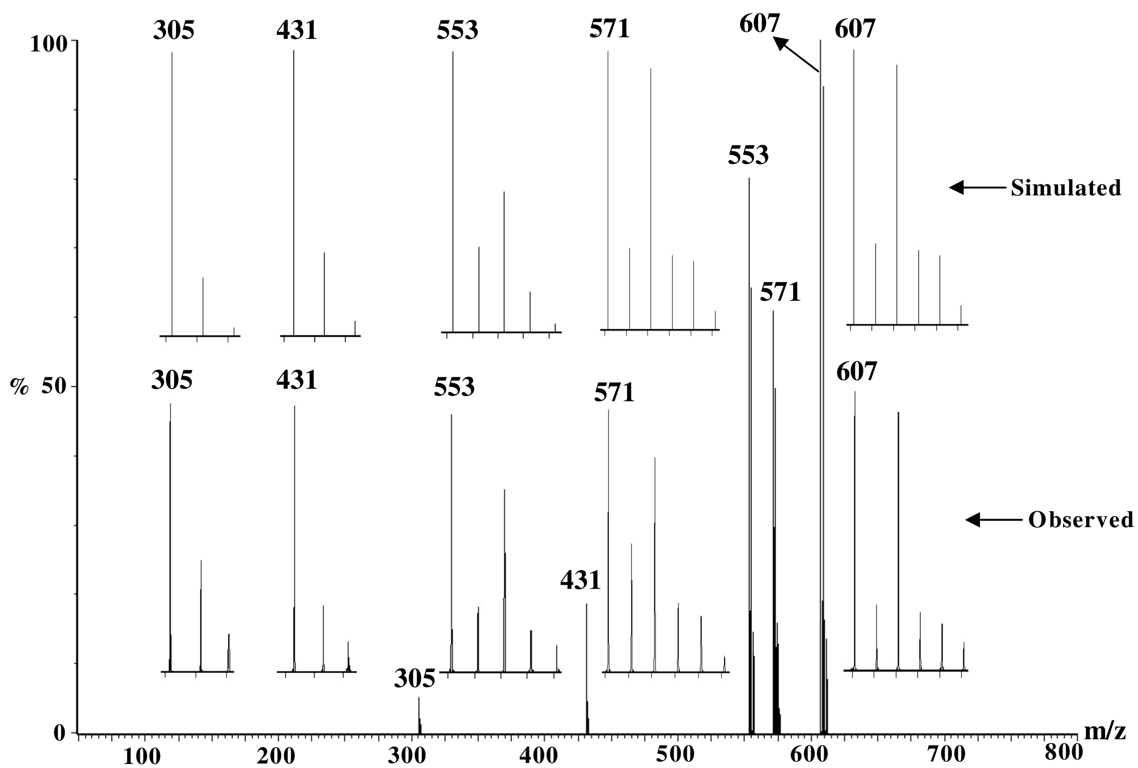

Fig. S6 Electrospray ionization mass spectrum (ESI-MS positive) of $[\{\{Cu^{II}_2L(\mu_{1,1}\text{-}N_3)\}_2(\mu_{1,1}\text{-}N_3)_2\}(\mu_{1,3}\text{-}N_3)_2]_n$ (**2**) in acetonitrile showing observed and simulated isotopic distribution patterns.

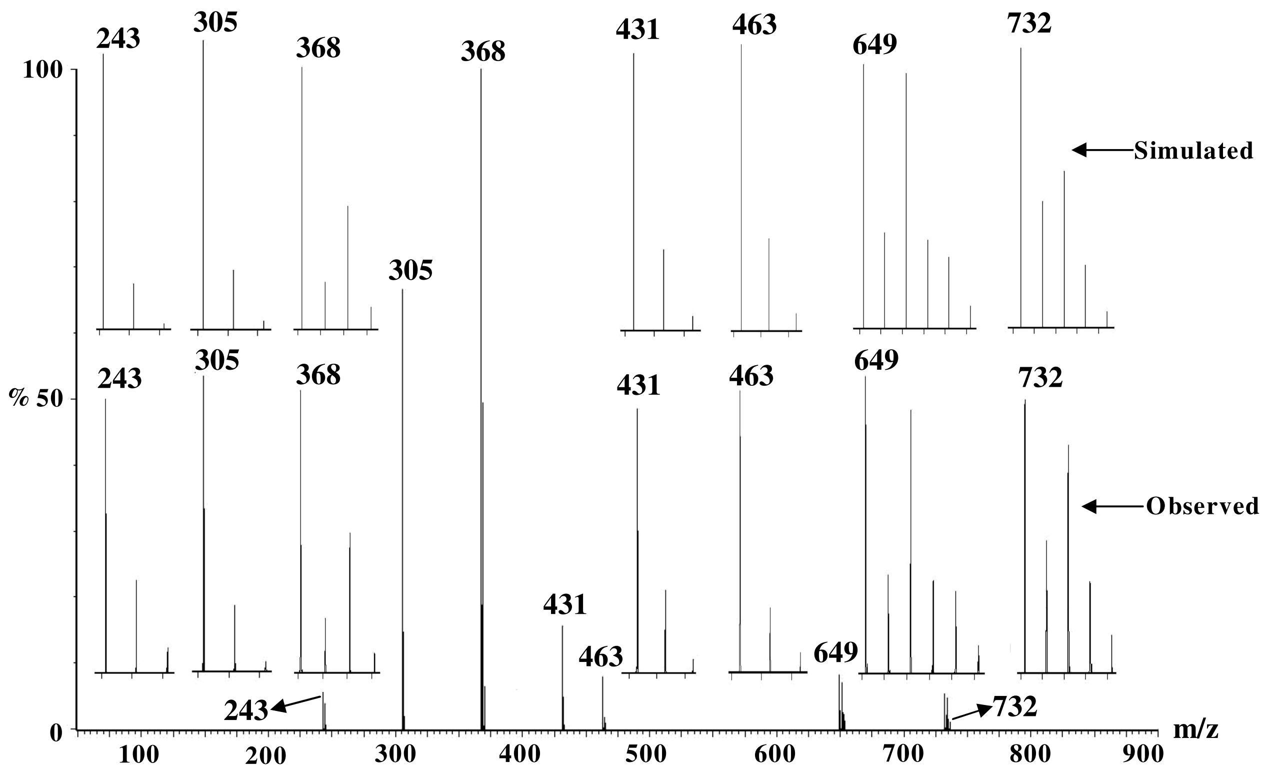

Fig. S7 Electrospray ionization mass spectrum (ESI-MS positive) of a 1:100 mixture of $[Cu_4L_2(\mu_3\text{-}OH)_2(NCO)_4].2H_2O$ (**1**) and 3,5-DTBCH$_2$ in acetonitrile, recorded after 10 minutes of mixing. Both the observed and simulated isotopic distribution patterns are shown.

Table S1 Representative examples copper(II) catalysts for catechol oxidase activity, along with their turnover numbers

Compound number	**Nuclearity**	K_{cat} **(h^{-1})**	**Reference**
A	Monocopper(II)	107.9	1*a*
B	Monocopper(II)	111	1*b*
C	Monocopper(II)	27.2	1*a*
D	Monocopper(II)	23.6	1*c*
E	Monocopper(II)	6.0	1*d*
F	Monocopper(II)	4.1	1*e*
G	Monocopper(II)	3.0	1*d*
H	Monocopper(II)	0.2	1*d*
J	Dicopper(II)	2804	2*a*
K	Dicopper(II)	1145	2*b*
L	Dicopper(II)	1127	2*c*
M	Dicopper(II)	900	2*d*
N	Dicopper(II)	236.5	2*e*
O	Dicopper(II)	214	2*f*
P	Dicopper(II)	189	2*g*
Q	Dicopper(II)	167.9	3*a*
R	Dicopper(II)	156.6	2*e*
S	Dicopper(II)	90	2*g*
T	Dicopper(II)	89.1	3*b*
U	Dicopper(II)	48	2*f*
V	Dicopper(II)	43	2*f*
W	Dicopper(II)	41.3	1*e*
X	Dicopper(II)	39.0	3*a*
Y	Dicopper(II)	33	2*f*
Z	Dicopper(II)	26.0	3*c*
AA	Dicopper(II)	23.2	1*e*
BB	Dicopper(II)	18.8	3*b*
CC	Dicopper(II)	12.5	3*d*
DD	Dicopper(II)	11.2	3*e*
EE	Dicopper(II)	3.2	1*e*
FF	Triicopper(II)	572.4	4*a*
GG	Triicopper(II)	80.3	4*b*
HH	Triicopper(II)	16.2	4*c*
JJ	Triicopper(II)	10.4	4*c*
KK	Triicopper(II)	7.5	1*e*
LL	Tetracopper(II)	39.9	3*a*
MM	Tetracopper(II)	19.4	4*c*
NN	Tetracopper(II)	15.8	4*c*
OO	Heptacopper(II) based one-dimensional	48.2	3*a*

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