

Electronic Supplementary Information

Nickel (II) di-aqua complex containing water cluster: Synthesis, X-ray structure and catecholase activity

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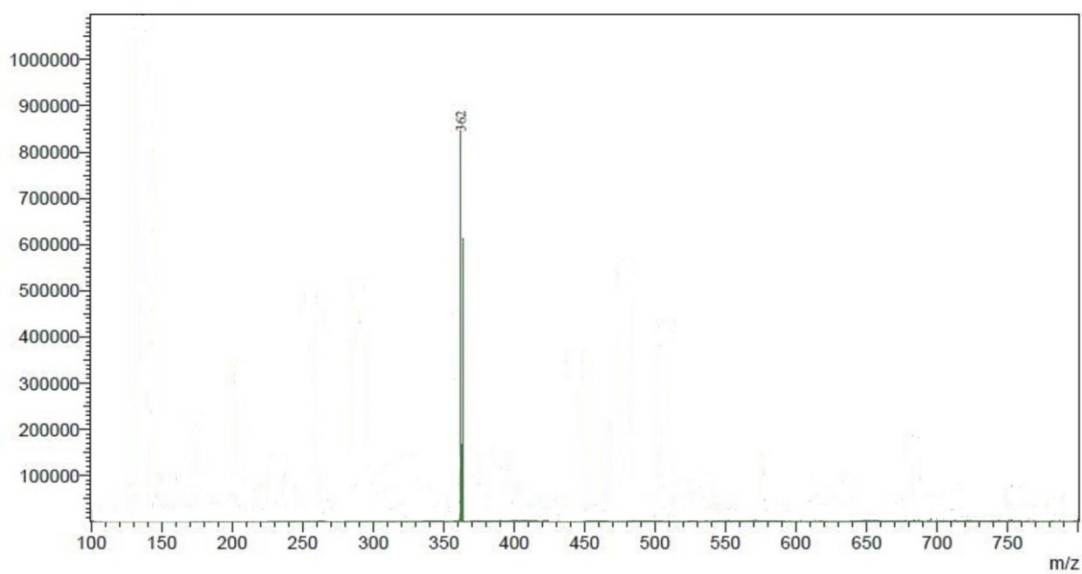


Fig. S1 Mass spectrum of **1.nH₂O** in MeOH.

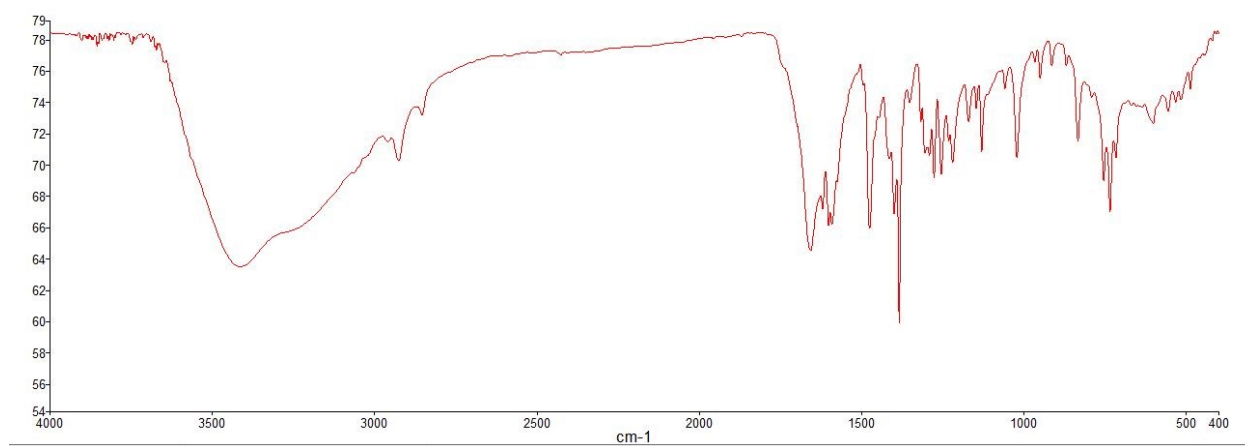


Fig. S2 Infrared spectrum of **1.nH₂O**.

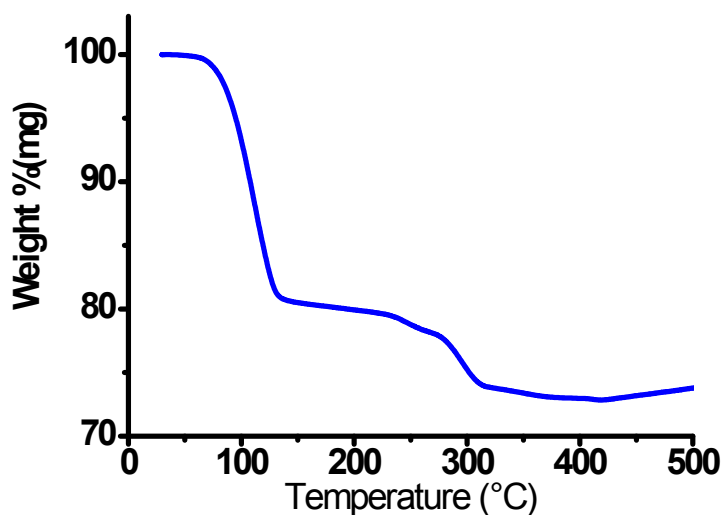


Fig. S3 Thermo gravimetric analyses of complex **1**.nH₂O.

Table S1. Hydrogen bond parameters for water in **1**.nH₂O

D - H...A	d(D-H)	D(H...A)	d(D..A)	<(D - H...A)
O140 --H141 ..O401	0.84(4)	1.88(4)	2.692(4)	160(4)
O140 --H142 ..O520	0.84(4)	1.92(4)	2.749(4)	171(4)
O230 --H231 ..O401	0.84(4)	1.90(4)	2.725(4)	167(4)
O230 --H232 ..O520	0.84(4)	1.98(4)	2.811(4)	170(4)
O240 --H241 ..O301	0.84(4)	1.89(5)	2.678(4)	156(6)
O240 --H242 ..O540	0.84(2)	1.99(3)	2.787(5)	159(4)
O330 --H331 ..O201	0.84(4)	1.92(4)	2.743(4)	165(4)
O330 --H332 ..O530	0.84(4)	2.00(4)	2.817(4)	167(5)
O340 --H341 ..O101	0.84(4)	1.87(4)	2.698(4)	169(5)
O340 --H342 ..O510	0.84(3)	1.92(3)	2.737(4)	166(4)
O430 --H431 ..O101	0.83(3)	1.93(4)	2.740(4)	163(4)
O430 --H432 ..O510	0.84(3)	1.95(3)	2.765(4)	162(4)
O440 --H441 ..O201	0.83(4)	1.89(4)	2.711(4)	169(4)
O440 --H442 ..O530	0.84(3)	1.96(4)	2.775(4)	163(4)
O510 --H511 ..O420	0.84(4)	1.85(4)	2.685(5)	173(5)
O510 --H512 ..O119	0.84(2)	2.11(2)	2.823(4)	143(3)

O520 --H521 ..O120	0.83(4)	1.92(4)	2.752(5)	175(3)
O520 --H522 ..O550	0.84(3)	1.88(4)	2.703(5)	166(6)
O530 --H531 ..O320	0.85(4)	1.92(4)	2.763(5)	171(5)
O530 --H532 ..O560	0.84(4)	1.94(4)	2.750(6)	163(5)
O570 --H571 ..O120	0.86(5)	1.94(6)	2.758(7)	158(7)
O570 --H572 ..O320	0.86(3)	1.92(4)	2.662(6)	144(8)

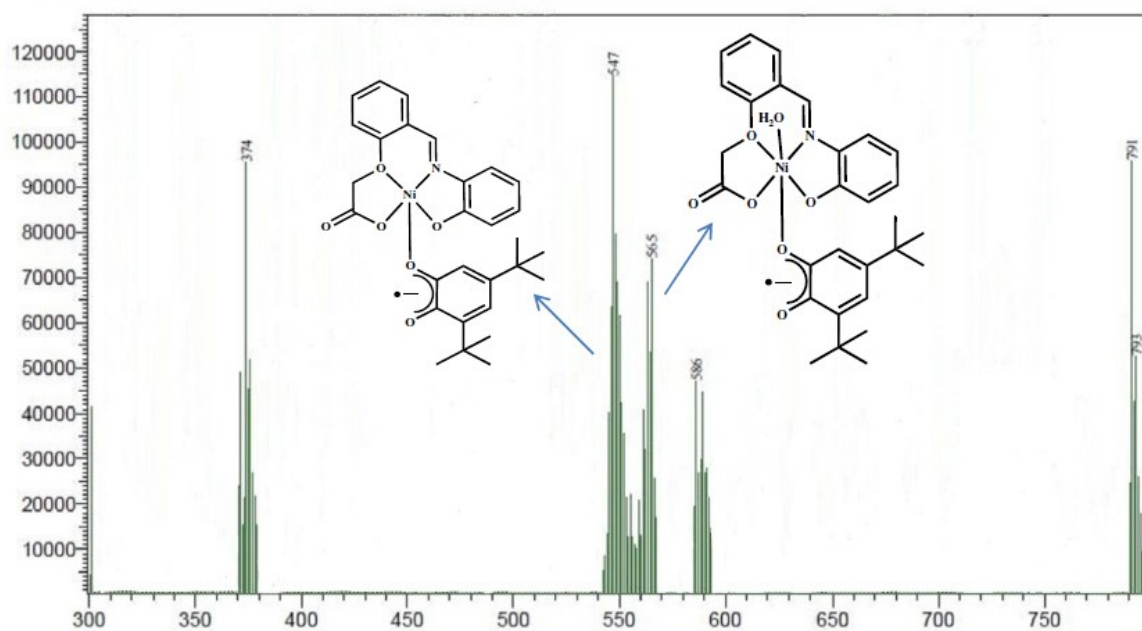


Fig.S4 Mass spectrum of **1**.nH₂O with 3,5-DTBC.

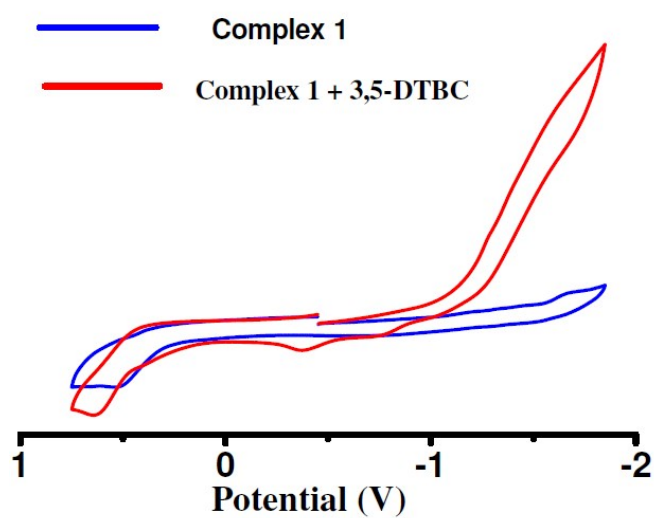


Fig. S5 Cyclic voltammogram of **1**.nH₂O in presence of 3,5-DTBC in CH₃CN (0.20 M [N(n-Bu)₄]PF₆) at 295 K.

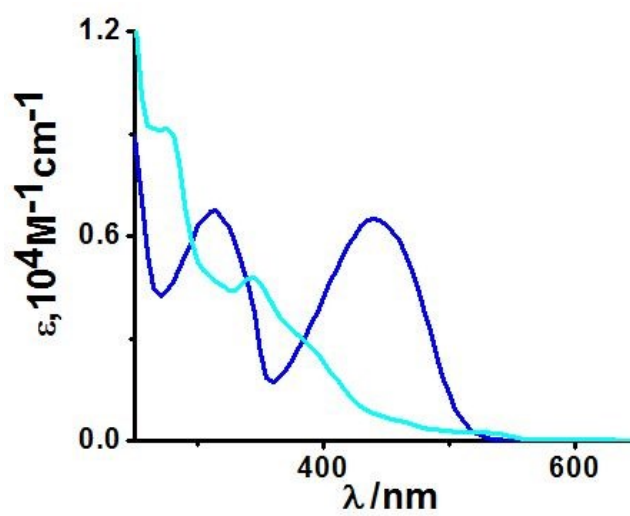


Fig. S6 UV-vis absorption spectra of (a) LH₂ (green) and (b) **1**.nH₂O (blue) in CH₃OH at 295 K.

Table S2. Electronic spectral data of LH₂ and **1**.nH₂O in CH₃OH at 295 K.

	λ_{max} (nm) (ϵ , $10^4 \text{ M}^{-1} \text{ cm}^{-1}$)
LH ₂	385(0.28), 335(0.68)
1 .nH ₂ O	440(3.73), 310(3.87)