



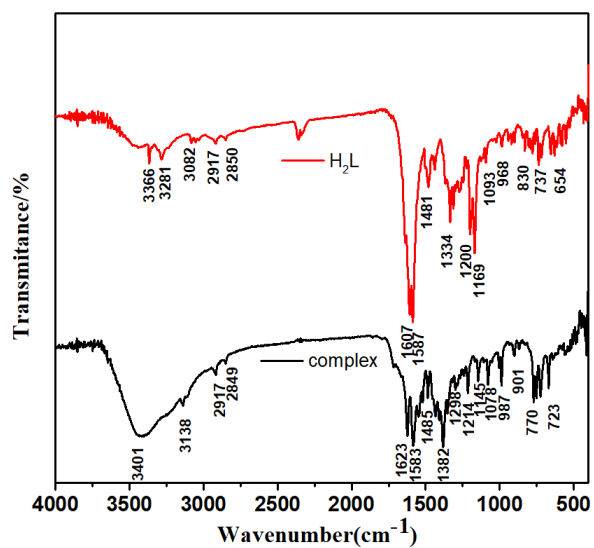
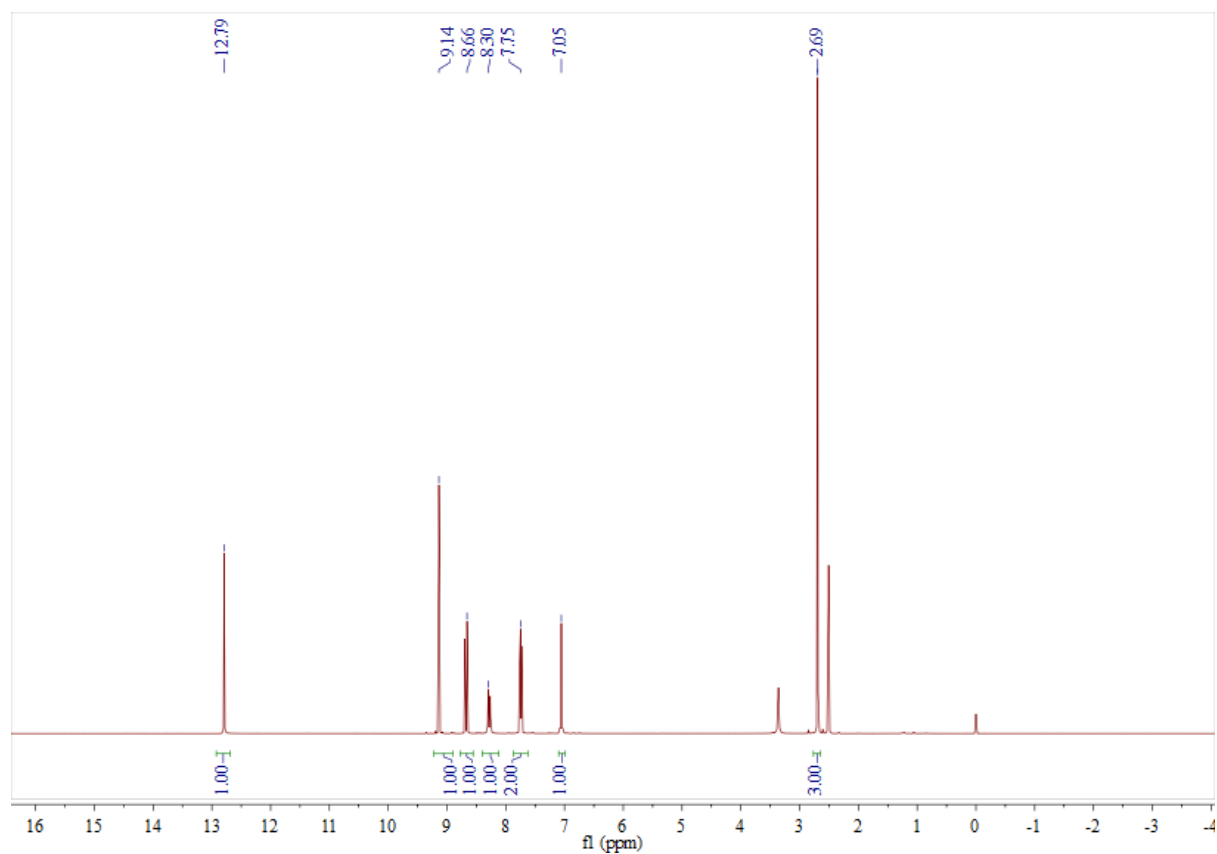
STRUCTURAL  
CHEMISTRY

**Volume 78 (2022)**

**Supporting information for article:**

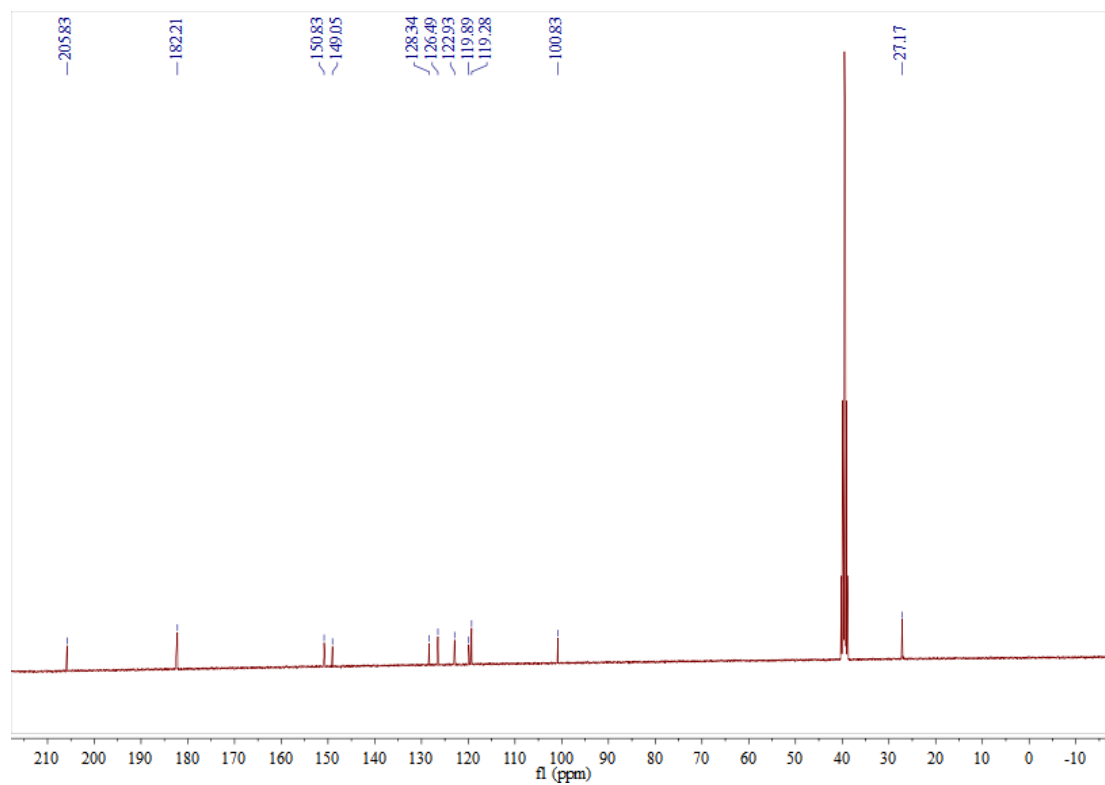
**Syntheses, crystal structures and Hirshfeld surface analysis  
of (Z)-3-[(3-acetyl-2-hydroxyphenyl)amino]-2-bromoprop-2-  
enal and a novel Zn<sup>II</sup> complex**

**Tan-Lin Jiang, Wei-Zhou Li, Qi-Feng Gao, Deng-Feng Tan, Jin-Ying Pang  
and Shu-Hua Zhang**

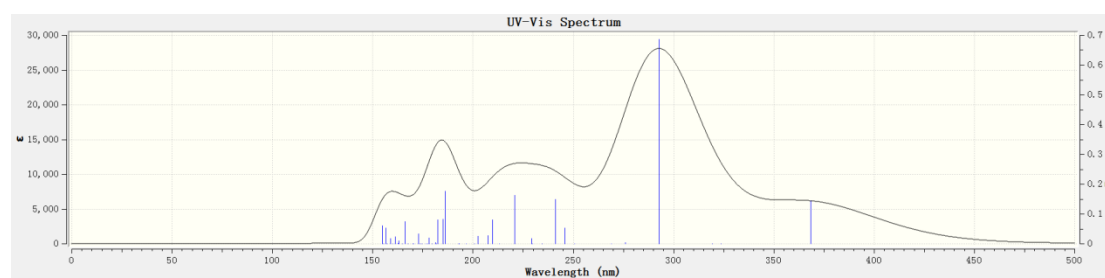
**Figure S1**The infrared spectra of H<sub>2</sub>L and **1**.**Figure S2**The <sup>1</sup>H-NMR spectra of H<sub>2</sub>L.

**Figure S3**

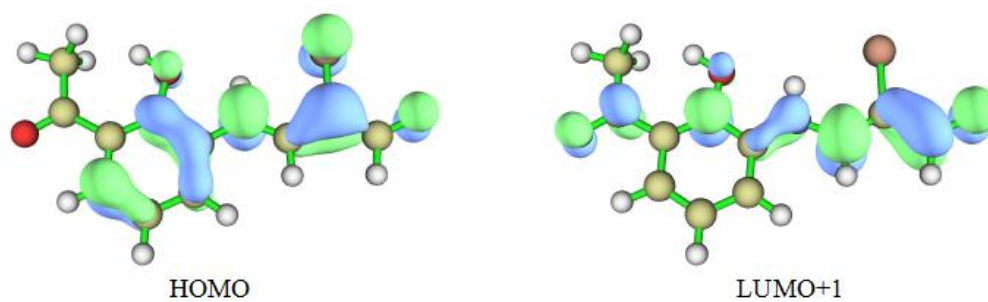
The  $^{13}\text{C}$ -NMR spectra of  $\text{H}_2\text{L}$ .

**Figure S4**

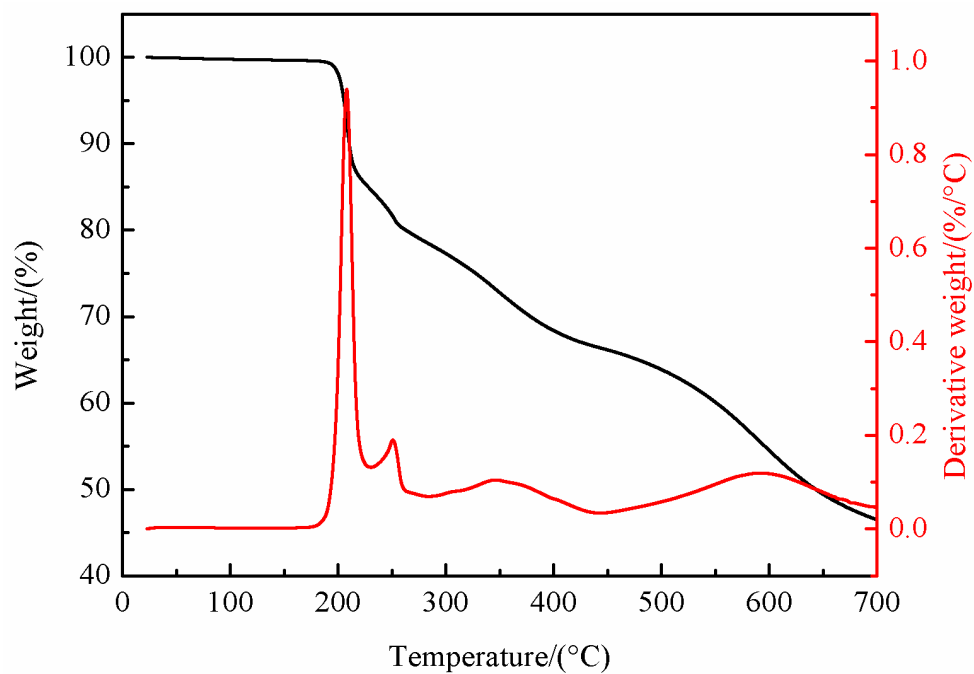
The Calculated UV-Vis spectrum of  $\text{H}_2\text{L}$ .

**Figure S5**

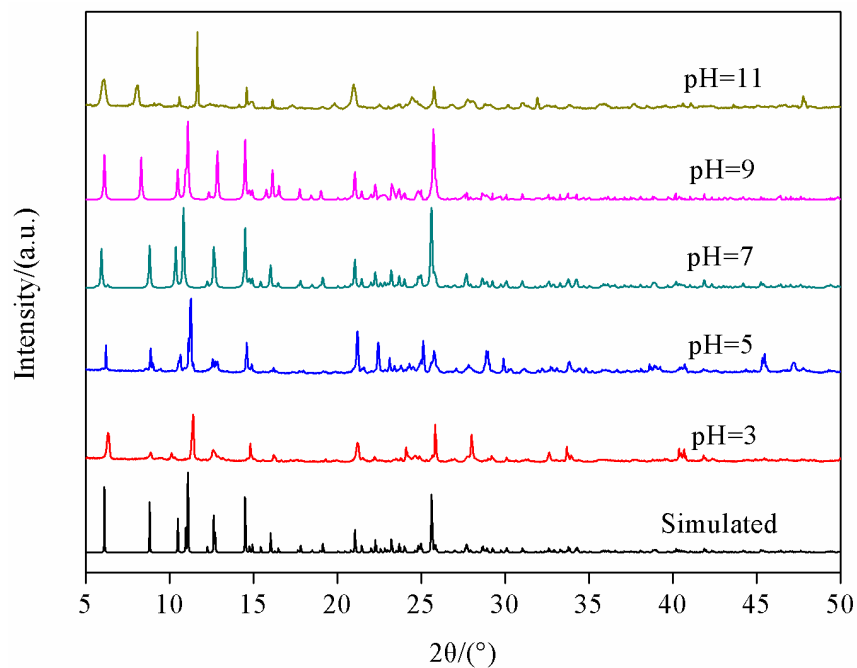
The molecular orbital diagram of  $\text{H}_2\text{L}$ .

**Figure S6**

The TG and DTG curves of the complex.

**Figure S7**

The experimental and simulated XRD curves of the complex.

**Table S1**

Bond order calculation results.

Chemical bond	Laplacian bond order	Mayer bond order
C3-N1	1.694	1.534
C2-C3	1.133	1.154
C4-N1	0.900	0.899

**Table S2**

Calculation results of coordination configuration.

Zn ions	PP-5	vOC-5	TBPY-5	SPY-5	JTBPY-5
Zn1	31.325	4.740	1.074	2.775	4.146

Zn2	56.461	41.125	36.973	38.884	43.903
-----	--------	--------	--------	--------	--------

Note:PP-5 = Pentagon; vOC-5 = Vacant octahedron; JTBPY-5 = Trigonal bipyramid; SPY-5= Spherical square pyramid; JTBPY-5= Johnson trigonal bipyramid J1