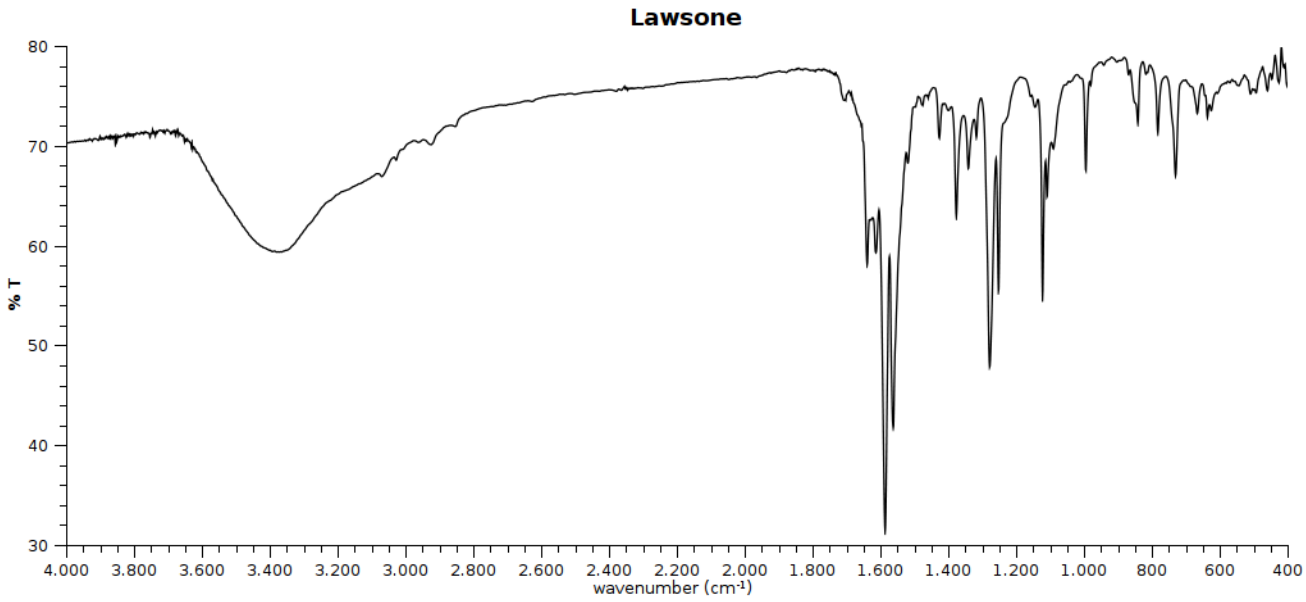
Supporting Information

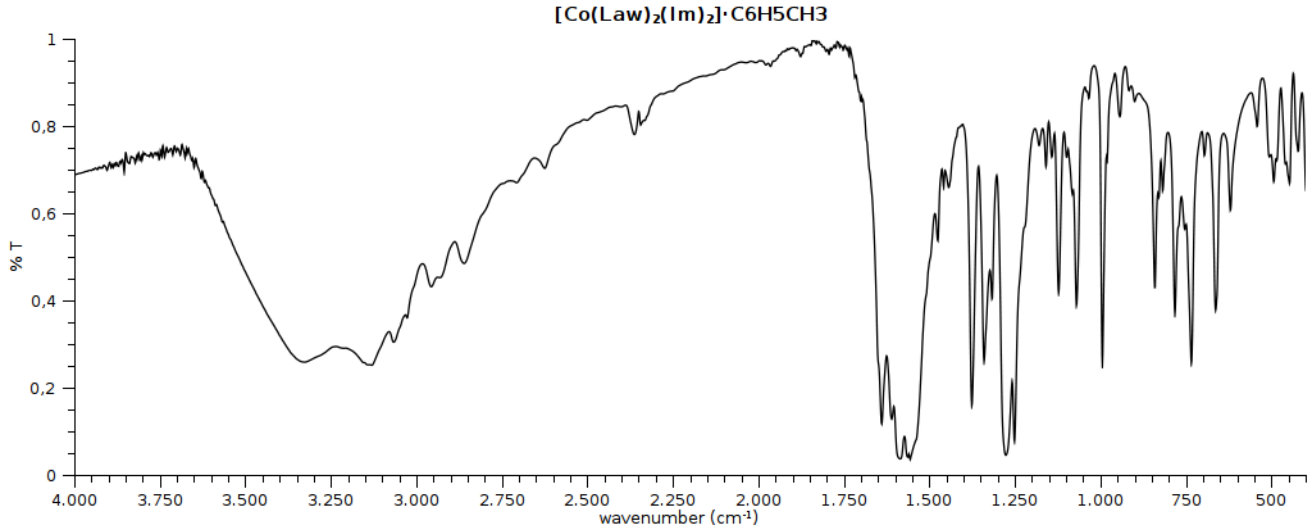
This document contents the Infrared spectra, Electronic Paramagnetic Resonance (EPR) spectra, calculated parameters for lawsone and lawsonate and figures of crystal structure with different representation of five compounds.

Infrared spectra – Except by the compound 2 all of spectra were collected on Perkin-Elmer FTIR spectrum GX using KBr pellets in the range of 4000-400 cm-1 with 4cm-1 of resolution. The compound 2 spectrum was collected on FTIR Perkin-Elmer One.

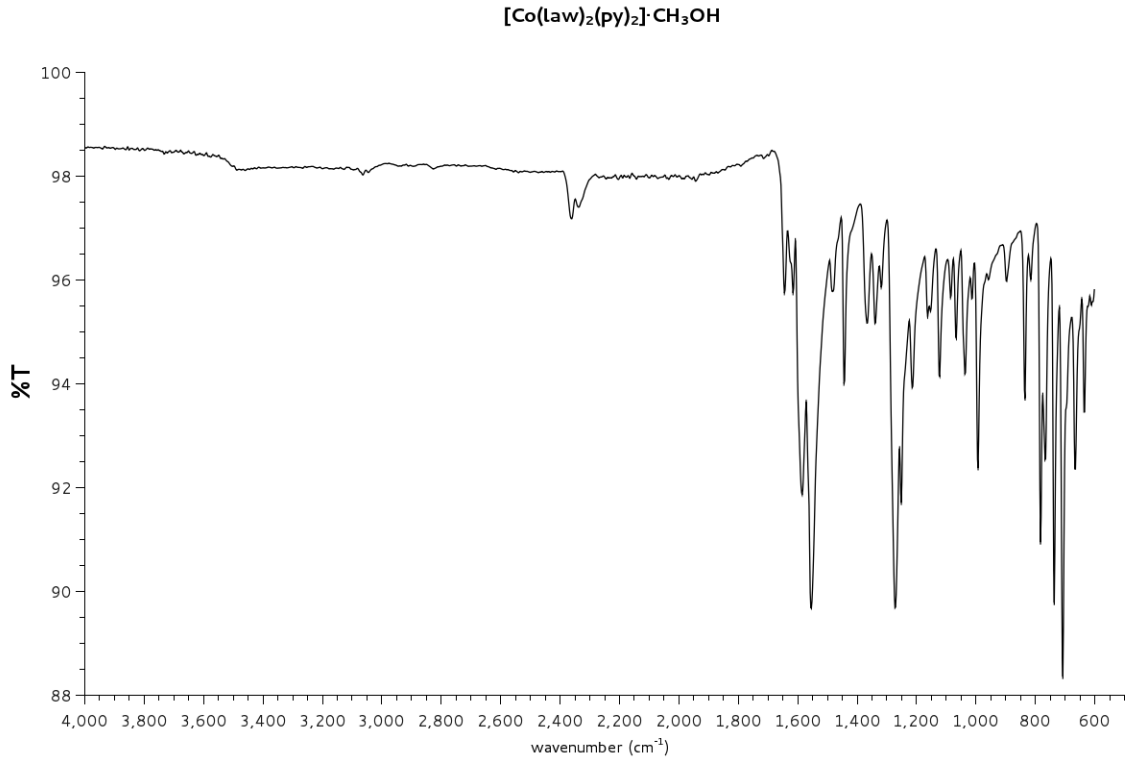
- Lawsone or 2-hidroxy-1,4-naphthoquinone



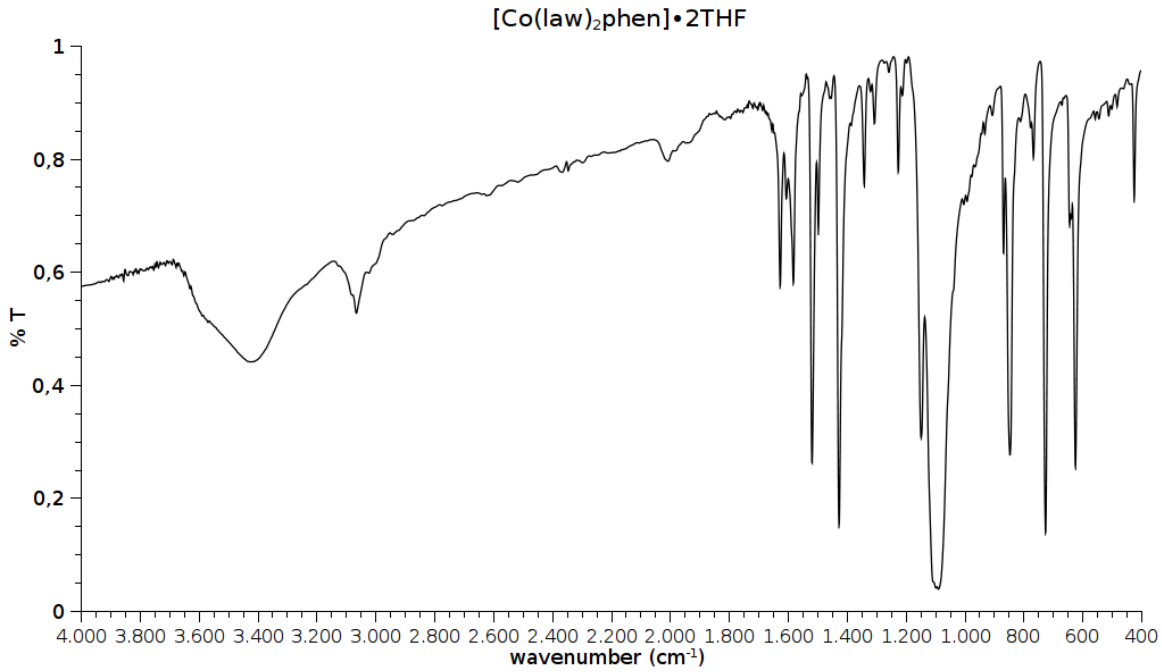
- Compound **1** - $[Co(Law)_2(Im)_2]\cdot C_6H_5CH_3$



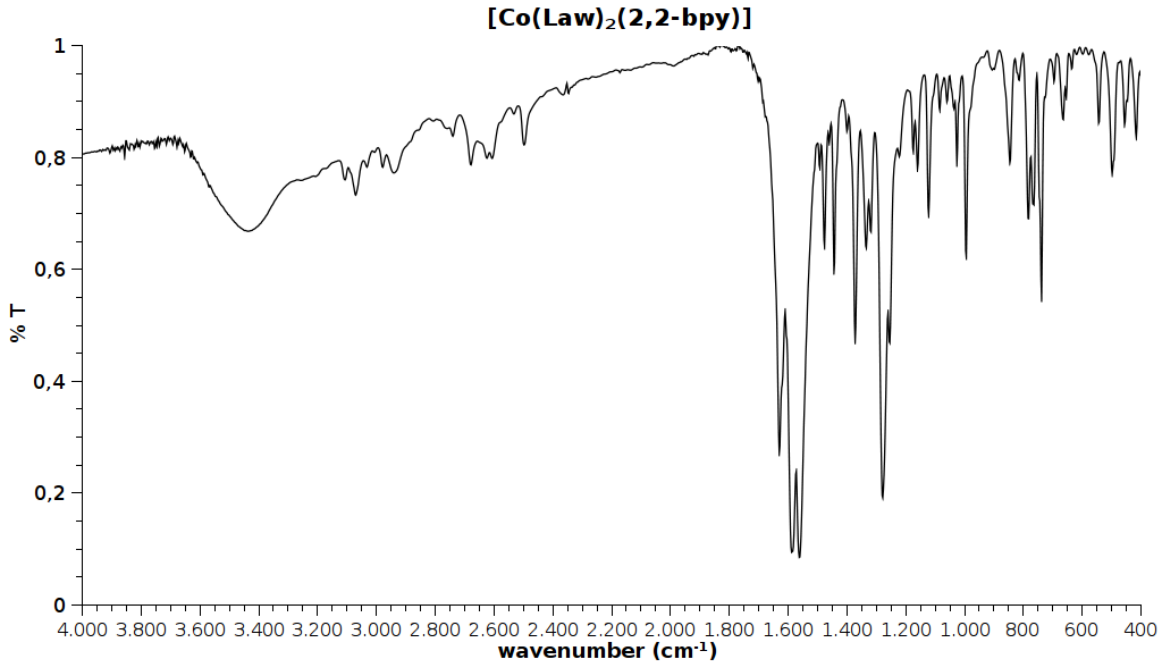
- Compound **2** - $[Co(law)_2(py)_2]\cdot CH_3OH$



- Compound **3**- $[Co(Law)_2(Phen)]\bullet 2(C_4H_8O)$



- [Co(Law)$_2$(2,2-bpy)]



Computational Methods - Ab initio calculations were performed with Firefly QC Package[i,ii], using DFT with base functions B3LYP/6-31+G. The optimization geometry of both the neutral

lawsone and lawsonate, were carried out. The following figures presents the bond lengths and bond angles in both structures.

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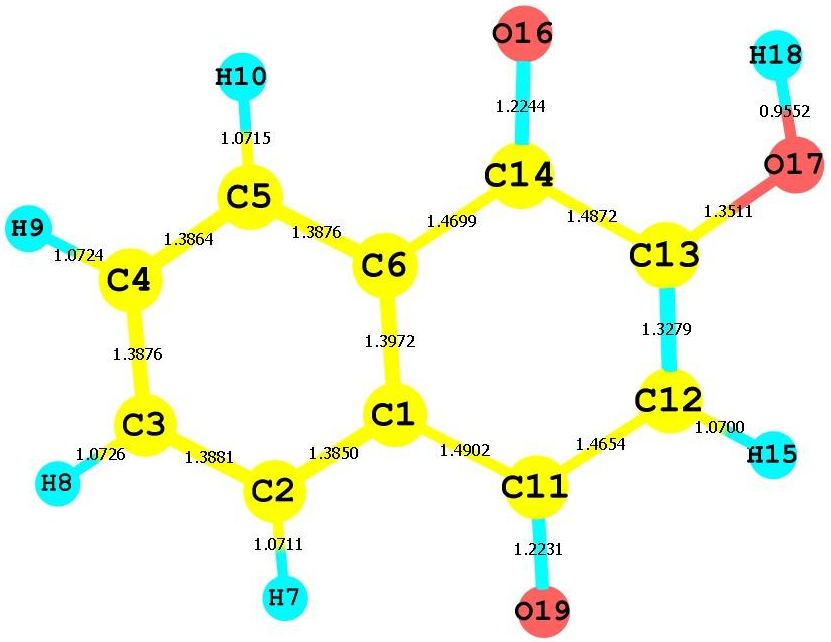
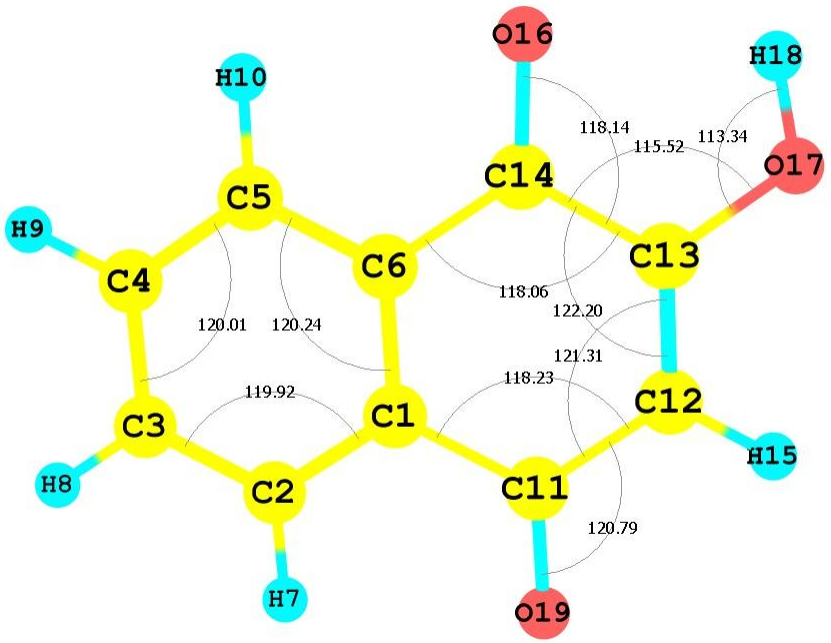
i Alex A. Granovsky, Firefly version 7.1.G, www.http://classic.chem.msu.su/gran/firefly/index.html

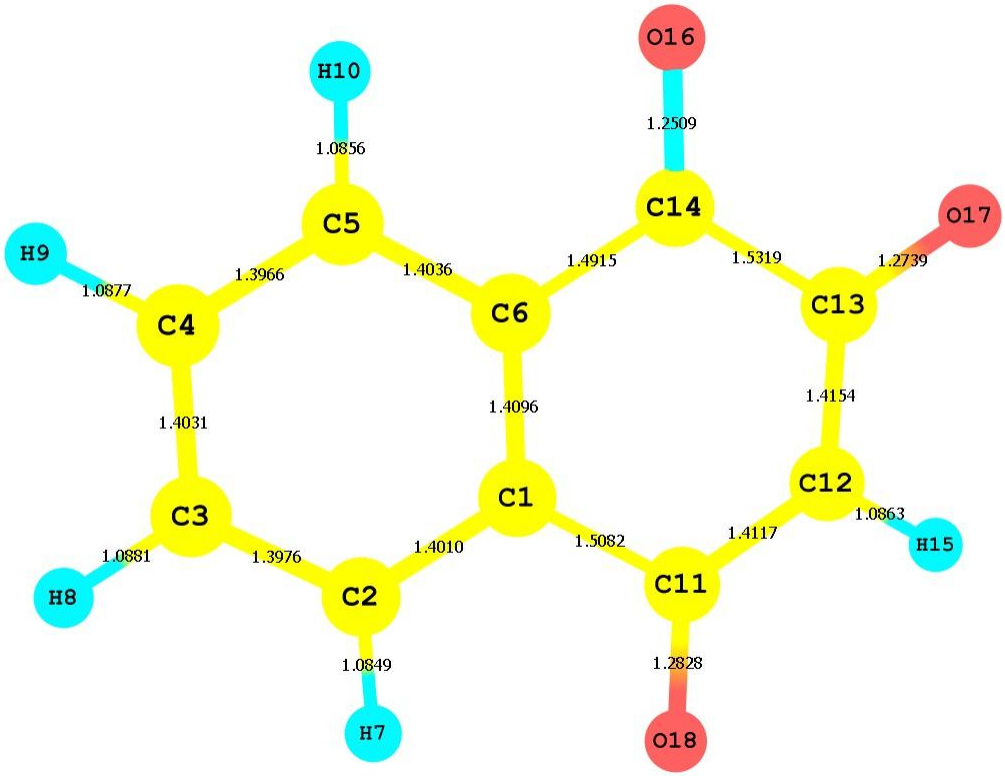
ii M.W.Schmidt, K.K.Baldridge, J.A.Boatz, S.T.Elbert, M.S.Gordon, J.H.Jensen, S.Koseki, N.Matsunaga, K.A.Nguyen, S.Su, T.L.Windus, M.Dupuis, J.A.Montgomery J.Comput.Chem. 14, 1347-1363 (1993).

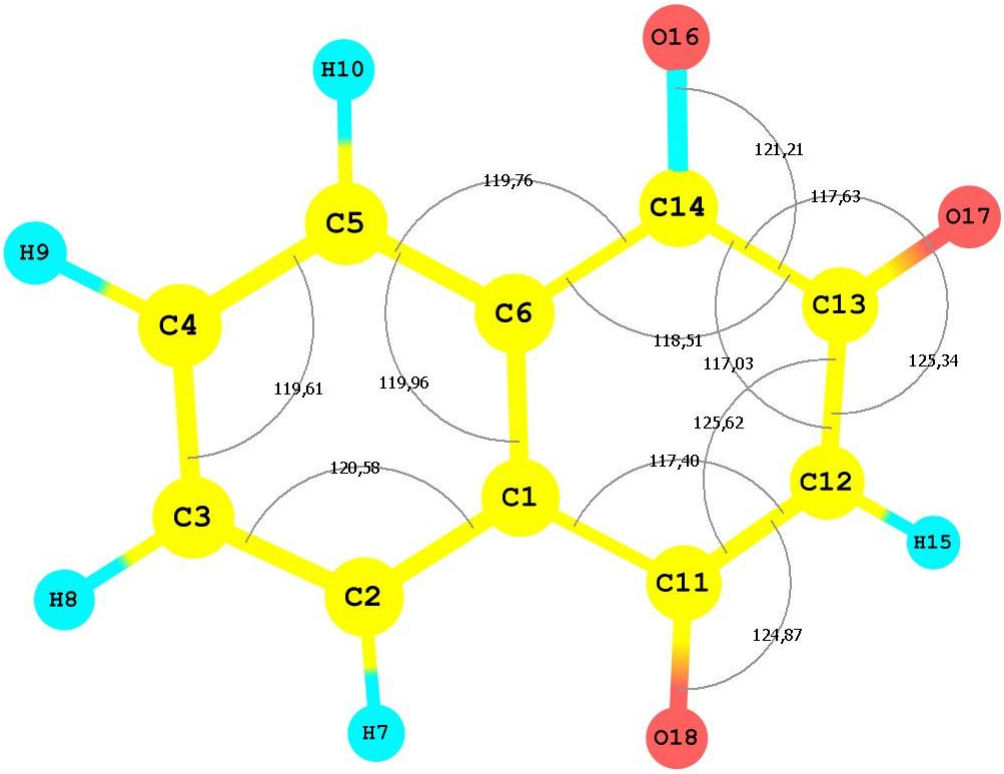
- Optimized Lawsone structure





- Optimized Lawsonate structure




O16
H10
121,21
119,76
C14
117,63
O17
C5
H9
C4
C6
C13
118,51
117,03
125,34
119,61
119,96
125,62
120,58
117,40
C12
C1
C3
H15
H8
C2
C11
124,87
H7
O18