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# Study of the conformational rearrangement of a tetradentate hydrazone ligand

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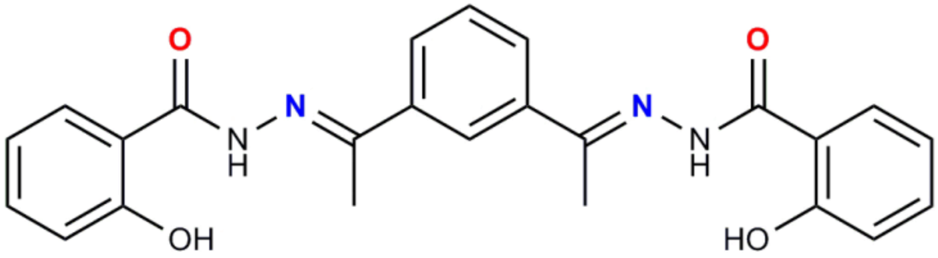
# The interest of this ligand molecule…

Hydrazones are very interesting molecules both in terms of their coordination chemistry and their wide range of biological applications.



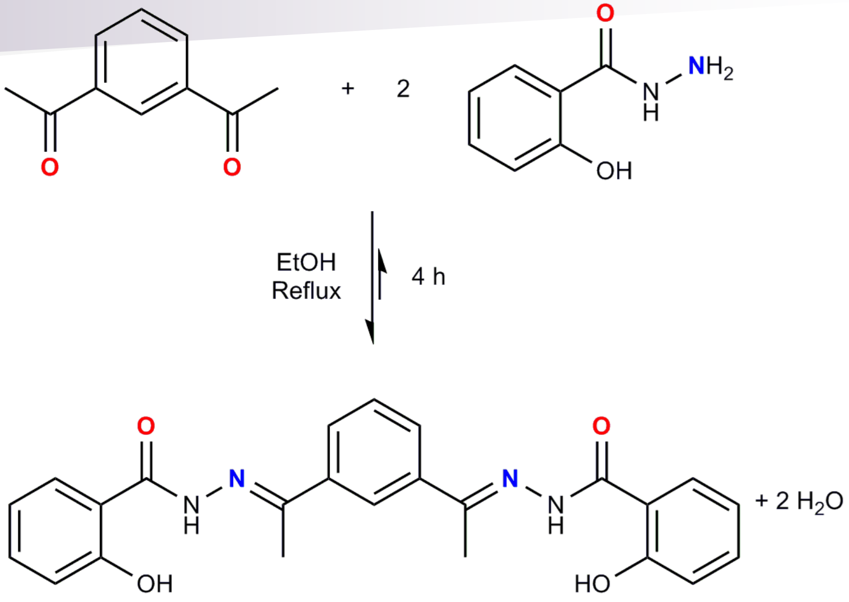
Hydrazone ligand $H_2L$

# Our aim…

The analysis of the conformations of this molecule together with the hydrogen bonding interactions allowed us to investigate the changes experienced by this ligand upon coordination to metal centers.

# Our strategy…

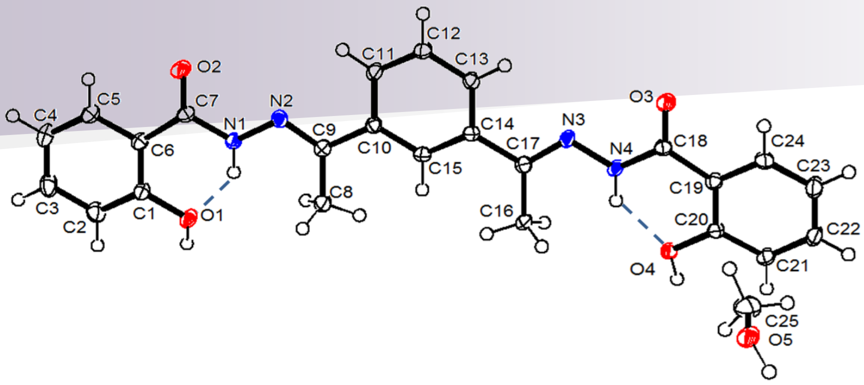
## Designing and Synthesis



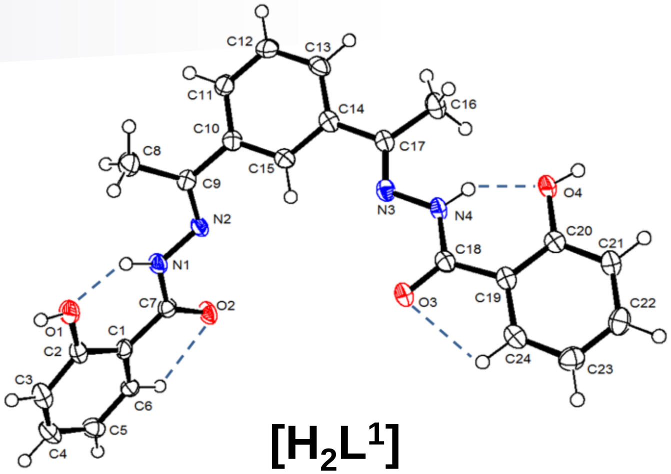
## Characterization (EA, MS ESI, IR, $^1$H NMR, X-ray diffraction)

**Ligand $H_2L$:** M.p. 162 ºC. Yield 0.50 g (90%). Elemental analysis, Calc. for $C_{24}H_{22}N_4O_4$: C, 67.0; H, 5.2; N, 13.0; O, 14.9. Found: C, 67.1; H, 5.1; N, 13.1; O, 14.7. MS ESI- (m/z): 429.2 ($[H_2L\text{-}H]^-$); IR (ATR, cm$^{-1}$): v(OH) 3440, v(NH) 3261, v(C=O) 1631, v(C=N) 1604, δ(NH) +v(N-CO) 1541, δ (NH)+v(CO) 1311. $^1$H NMR (DMSO-$d_6$, ppm), δ (m, nH): 11.82 (s, 2H), 11.38 (s, 2H), 8.31 (s, 1H), 8.01 (d, 2H, J= 7.5 Hz), 7.90 (d, 2H, J= 7.3 Hz), 7.52 (t, 1H, J= 7.5 Hz), 7.42 (t, 2H, J= 7.3 Hz), 7.02-6.99 (m, 2H+2H), 2.30 (s, 6H), 2.37 (s, 6H).

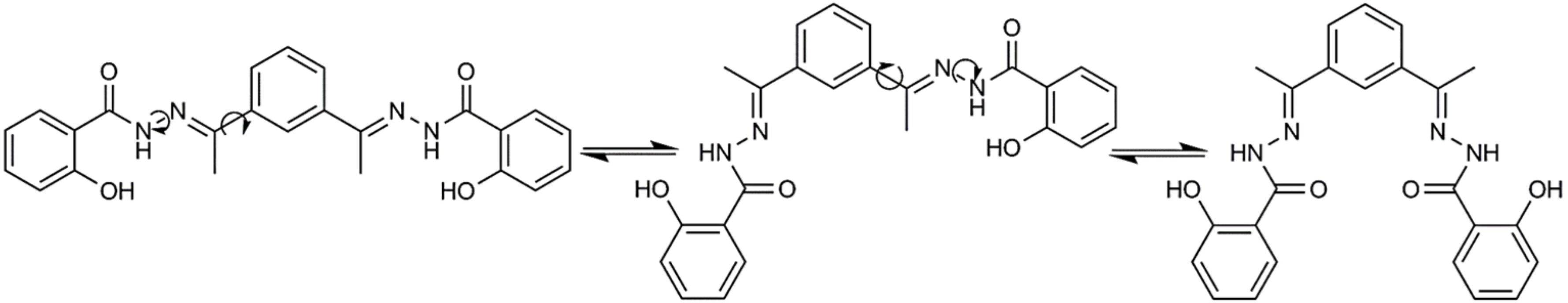
# Our results…



$[H_2L^1]\cdot MeOH$



$[H_2L^1]$



*syn-open*

*anti-open*

*syn-close*

# Our conclusions…

This is the first example of a tetradentate hydrazone ligand structurally studied.

Of particular interest is the study of the conformation of the free ligand in the solid state to establish comparisons with that required to form a metal complex.

The syn-open arrangement of $H_2L$ (**1**) would be suitable for the coordination of two units of ligand to two metal centers without crossing, thus yielding a mesohelical-type complex.

In case **2,** the ligand molecules adopt a syn-close type conformation, which would be suitable for direct coordination of the $N_2O_2$ donor set to the same metal ion.