

## Electronic Supplementary Information (ESI)

### Synthesis and X-ray structure of a novel organometallic trinuclear oxido-imido iridium complex

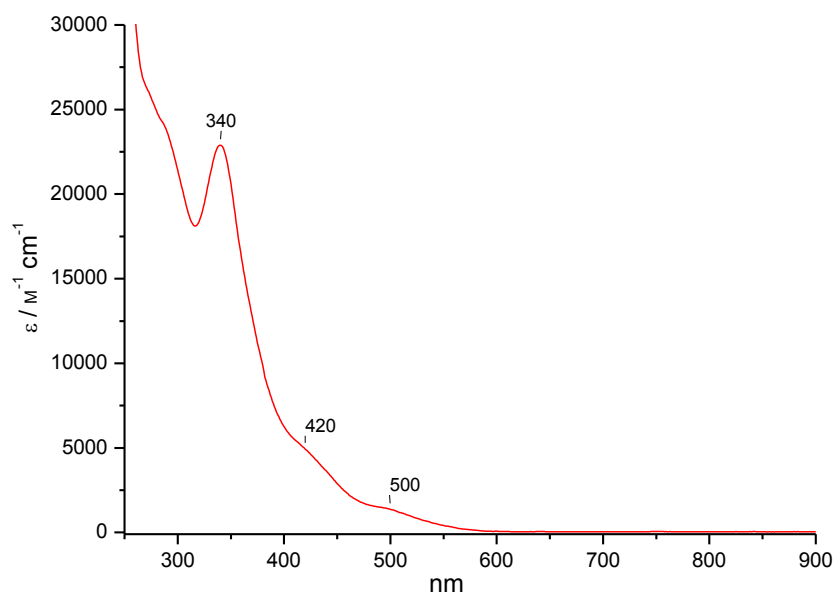
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#### Contents

1. UV-vis spectroscopy
2. Mass spectrometry
3. NMR spectroscopy

#### 1. UV-vis spectroscopy

UV-vis spectra were recorded on a Perkin-Elmer, Lambda 2 UV-vis spectrophotometer in dichloromethane.



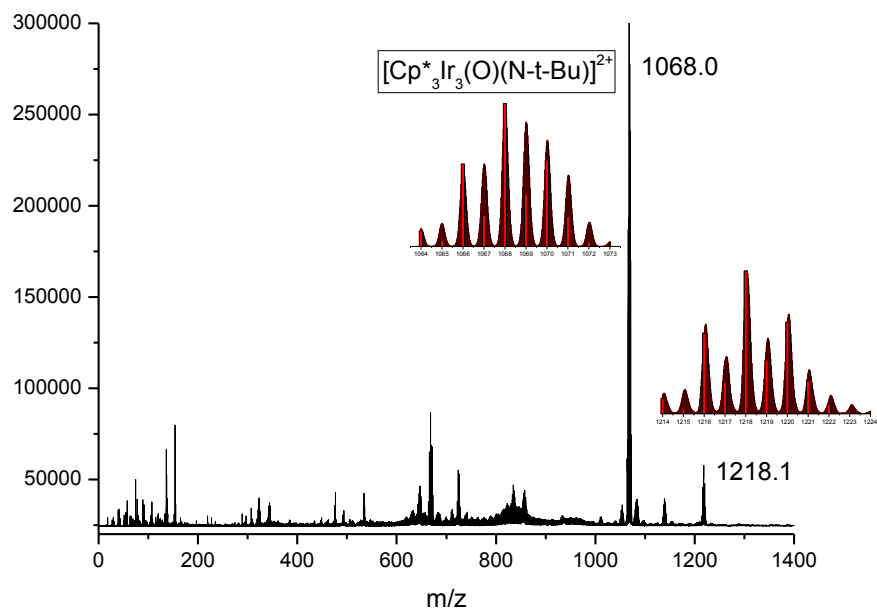
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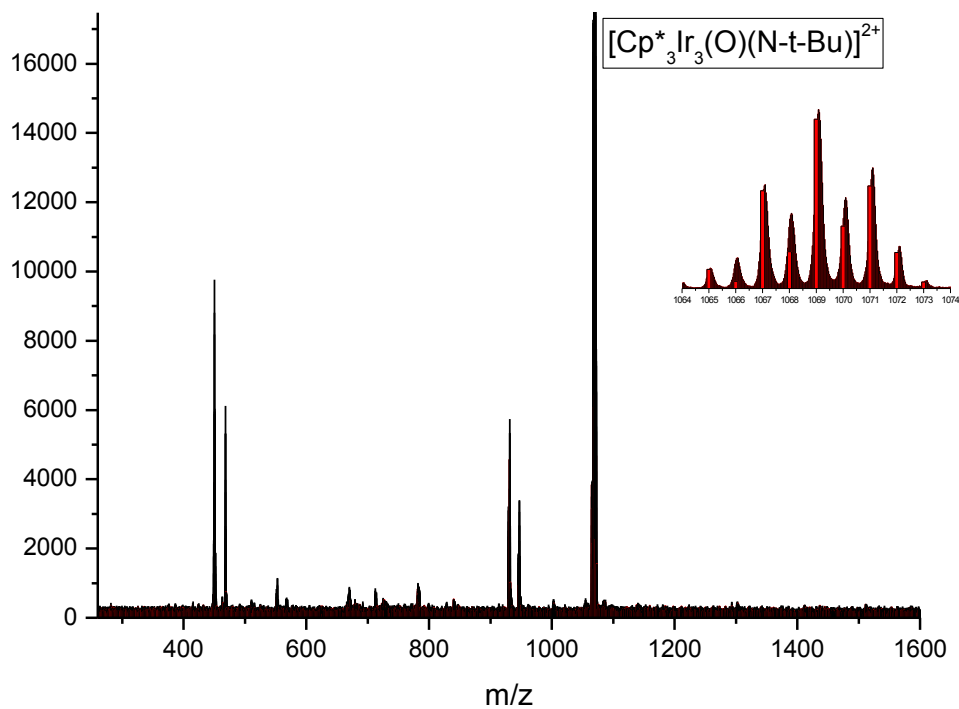
‡ CCDC 793862 (1) and CCDC 793863 (2) contains the supplementary crystallographic data for this paper.

## 2. Mass spectrometry

FAB+ spectra were recorded on a Jeol JMS-HX 110 tandem mass spectrometer using *m*-nba as matrix. Inserts show the calculated mass spectrum: 1068.0 {M-H}<sup>+</sup>, 1218.1 {M+OTf}<sup>+</sup>



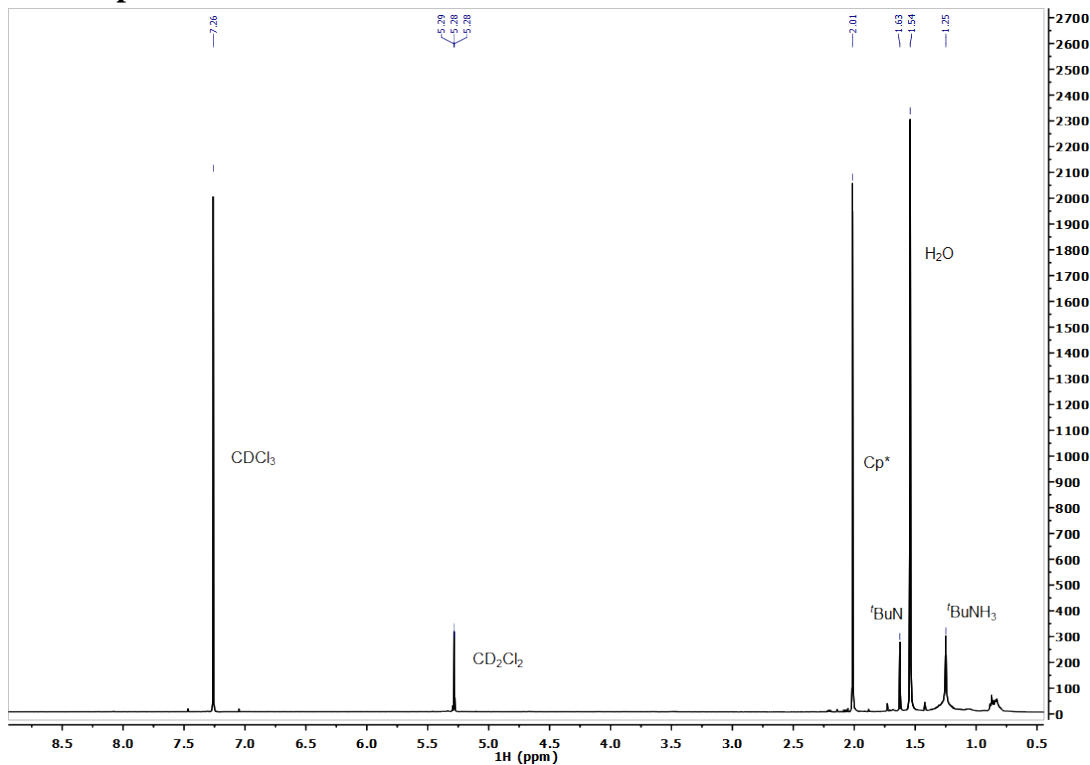
MALDI+ spectra were recorded on a Micromass Q-ToF (ESMS), Bruker Daltronics Autoflex mass spectrometer using dithranol as matrix. Inserts show the calculated mass spectrum: 1069.0 {M}<sup>+</sup>



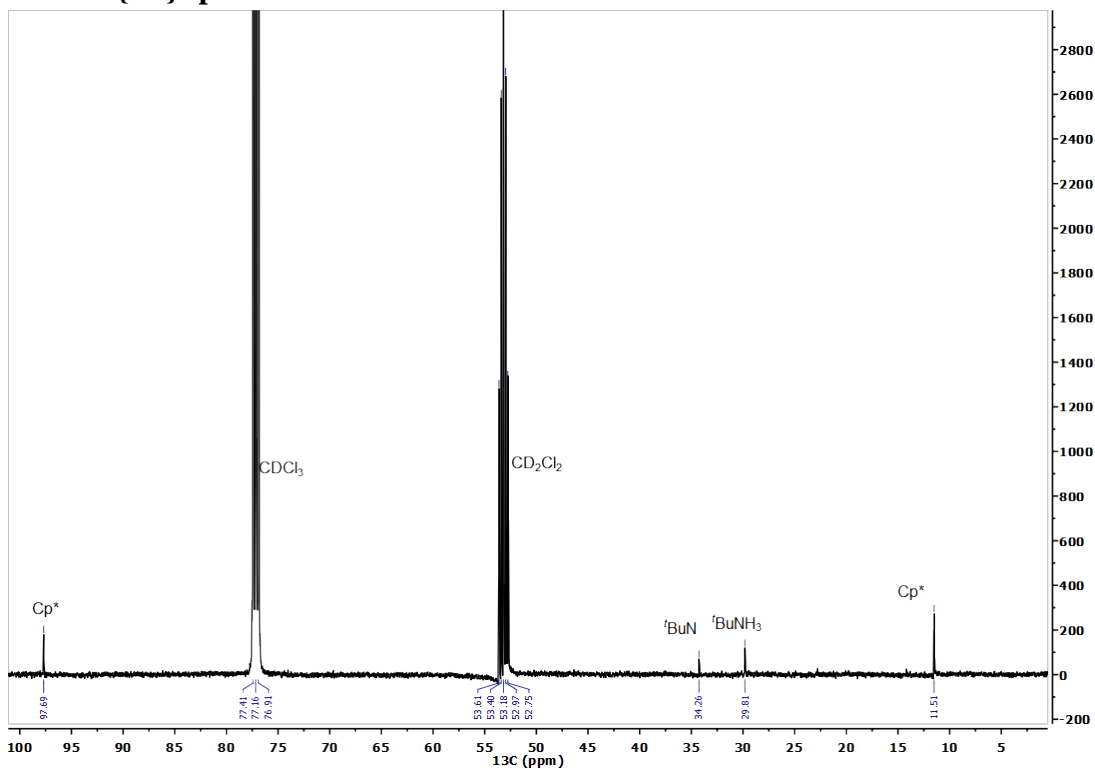
### 3. NMR spectroscopy of $(t\text{-BuNH}_3)[\text{Cp}^*\text{Ir}_3(\mu_3\text{-O})(\mu_3\text{-N}^t\text{Bu})](\text{O}_3\text{SCF}_3)_3 \cdot \text{CH}_2\text{Cl}_2$ (1).

$^1\text{H}$ ,  $^{13}\text{C}\{-^1\text{H}\}$  and HSQC NMR spectra were recorded on a Bruker 500 MHz spectrometer equipped with a cryo probe in  $\text{CDCl}_3$  with 10%  $\text{CD}_2\text{Cl}_2$

#### 3 a. $^1\text{H}$ spectrum



#### 3 b. $^{13}\text{C}\{-^1\text{H}\}$ spectrum



### 3 c. $^{13}\text{C}$ - $^1\text{H}$ HSQC spectrum

