*Title:* **Co-crystallization of dicyandamide and copper (II) salts for agrochemical applications**

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The objective of this thesis is to synthesise a co-crystal that can inhibit the enzymes *Urease* and *AMO*. These two enzymes are responsible for the degradation of urea when it is applied as a fertiliser in the soil, which leads to contamination and loss of nitrogen. The purpose was to inhibit these enzymes to improve the effectiveness of urea fertilisers. The components forming the co-crystal are copper (II) salts ($Cu(NO_3)_2$ and $CuCl_2$ ) for the inhibition of *Urease* and dicyandamide (DCD), for the inhibition of *AMO*.

Both co-crystals had been reported in the literature, but it was unclear which method was used to synthesis them. Moreover, I investigated if different structures existed. In this work I used two typical methods of crystal engineering: ball-milling and slurry.

For the characterization, I used X-Ray Powder diffraction, thermogravimetric analysis, differential scanning calorimetry and the software EXPO2014 for the structure resolution.

For the co-crystal with $DCD_2$-$Cu(NO_3)_2$, it was found that the co-crystal obtained through ball-milling, $DCD_2$-$Cu(NO_3)_2$ -$4H_2O$, has the same structure as the compound found in the literature, see Figure 1. And the co-crystal obtained through slurry has a different structure with two less water molecules, $DCD_2$-$Cu(NO_3)_2$ -$2H_2O$, see Figure 2.

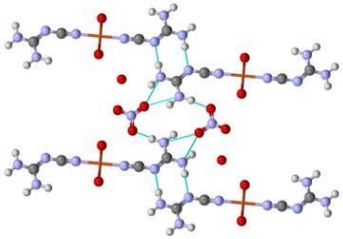

Figure 1. $DCD_2$-$Cu(NO_3)_2$-$4H_2O$ structure obtained through ball-milling.

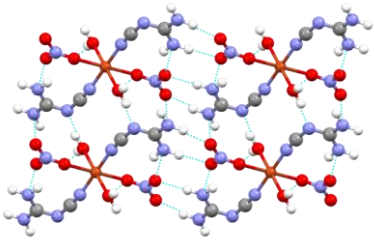

Figure 2. $DCD_2$-$Cu(NO_3)_2$ -$2H_2O$ structure obtained through slurry.

For the co-crystal with $DCD_2$-$CuCl_2$, it was found that the co-crystal obtained through ball-milling, $DCD_2$-$CuCl_2$ -$2H_2O$, has the same structure as the compound found in the literature, see Figure 3. And the co-crystal obtained through slurry has a different crystal structure with the same water molecules, $DCD_2$-$CuCl_2$ -$2H_2O$, see Figure 4.

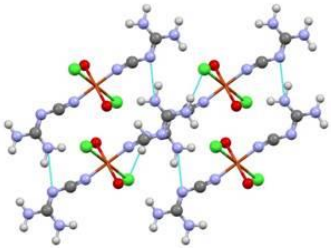

Figure 3. $DCD_2$-$CuCl_2$ -$2H_2O$ structure obtained through ball-milling.

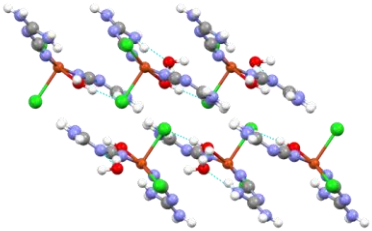

Figure 4. $DCD_2$-$CuCl_2$ -$2H_2O$ structure obtained through slurry.