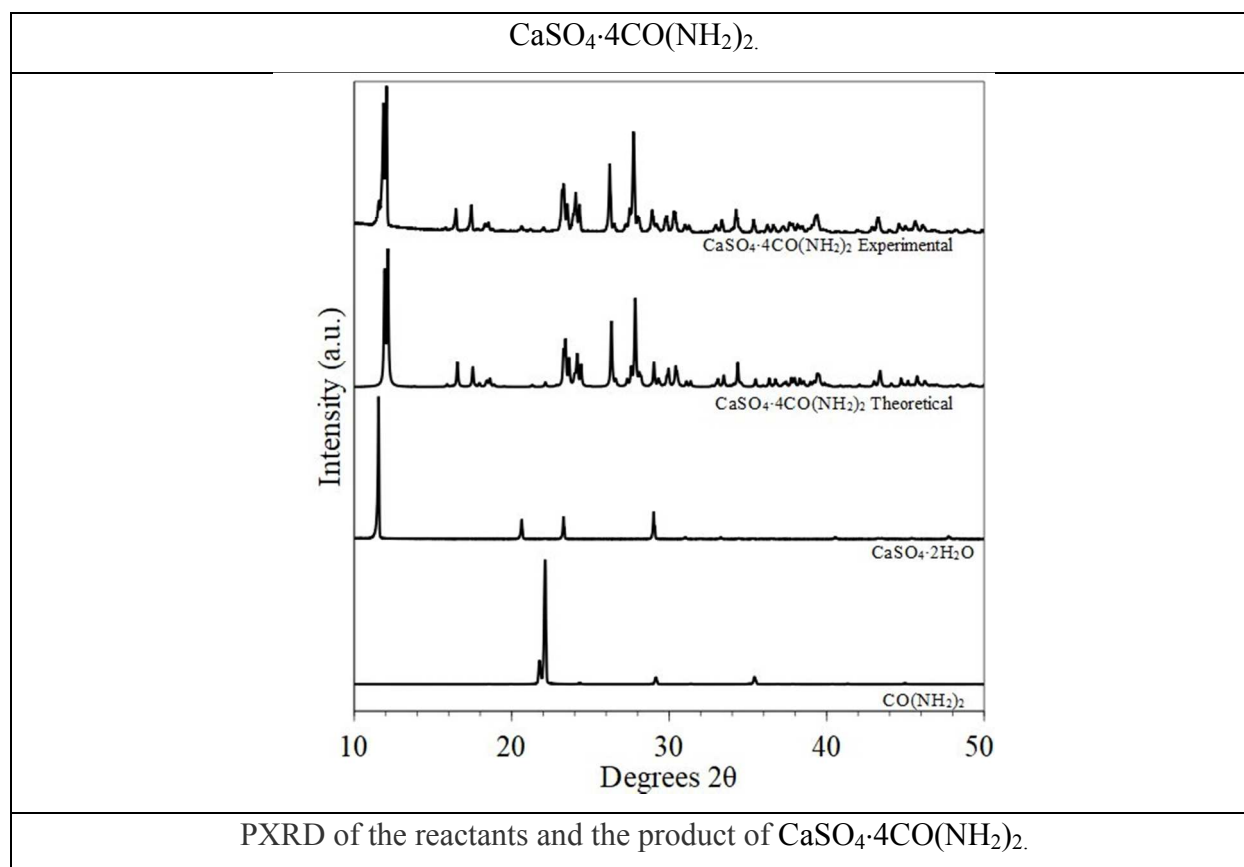


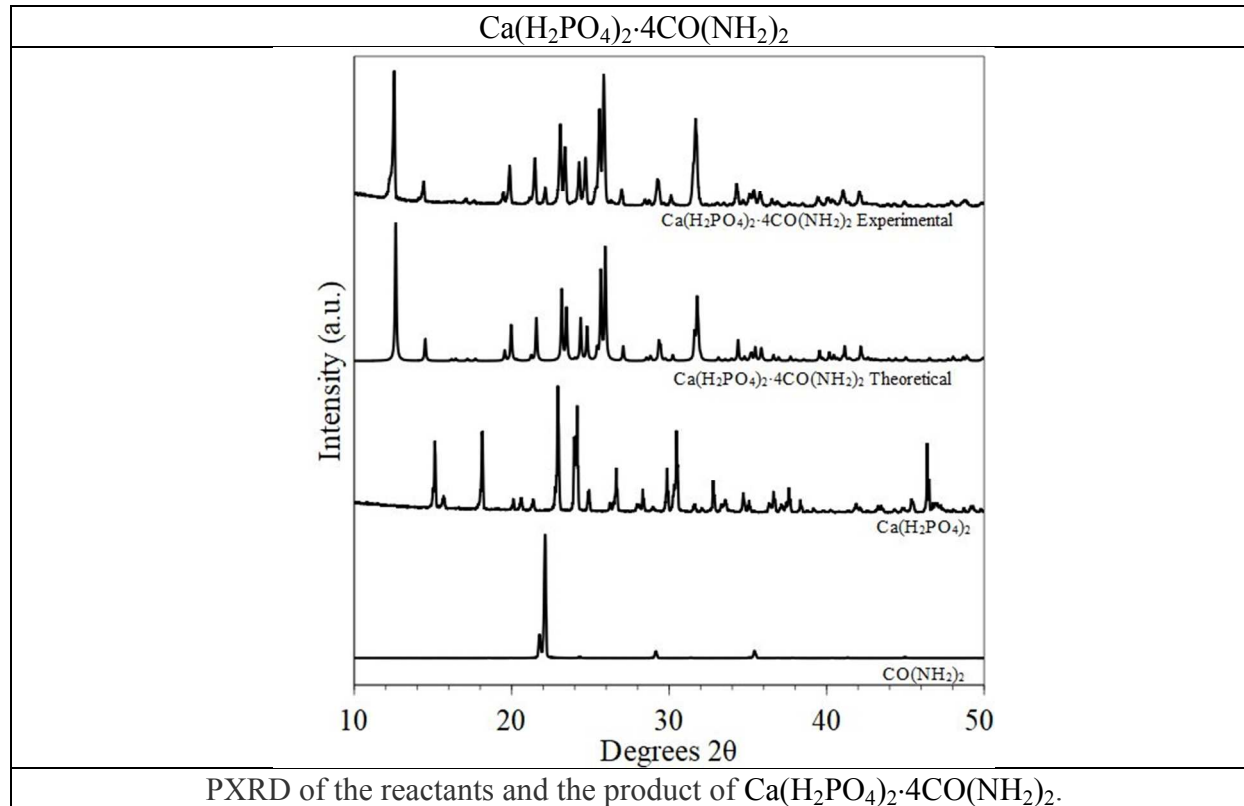
**Mechanosynthesis of magnesium and calcium salt-urea ionic cocrystal fertilizer materials  
for improved nitrogen management**

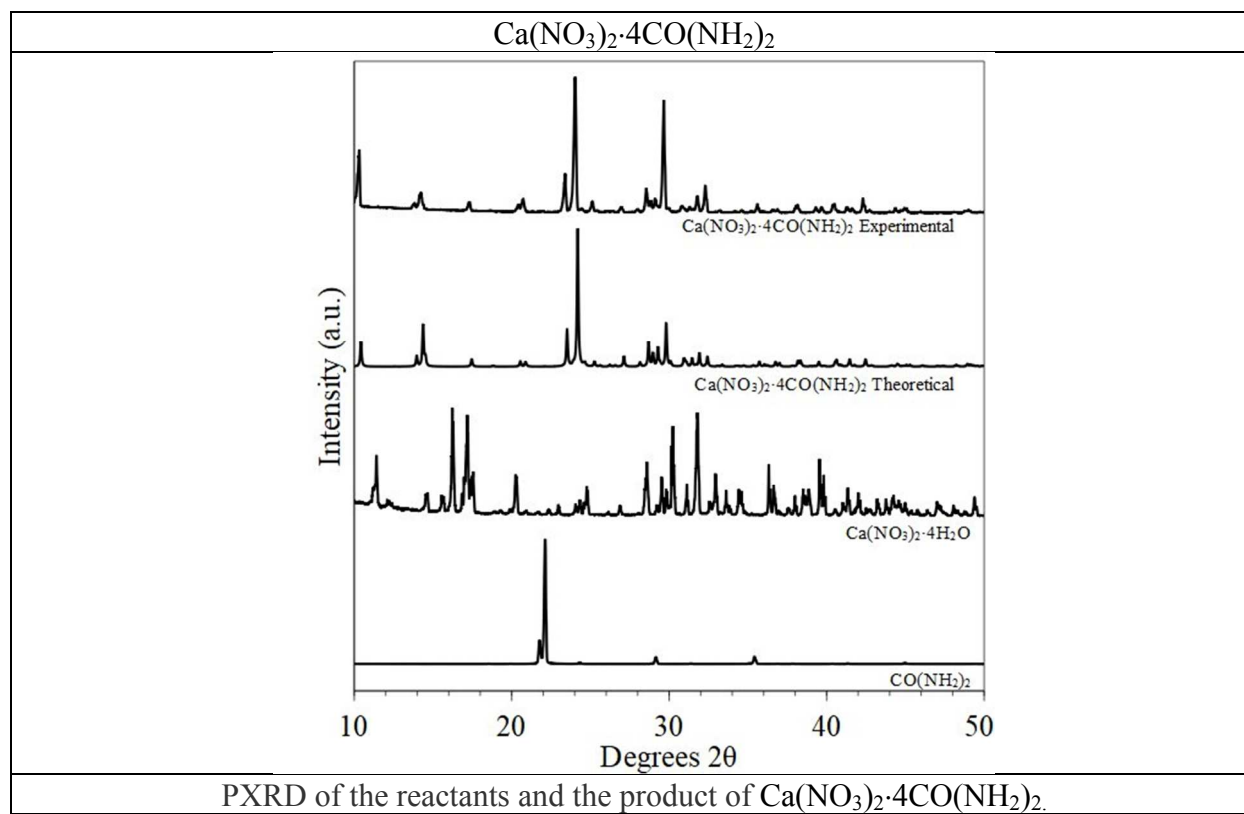
Kenneth Honer, Eren Kalfaoglu, Carlos Pico, Jane McCann and Jonas Baltrusaitis \*

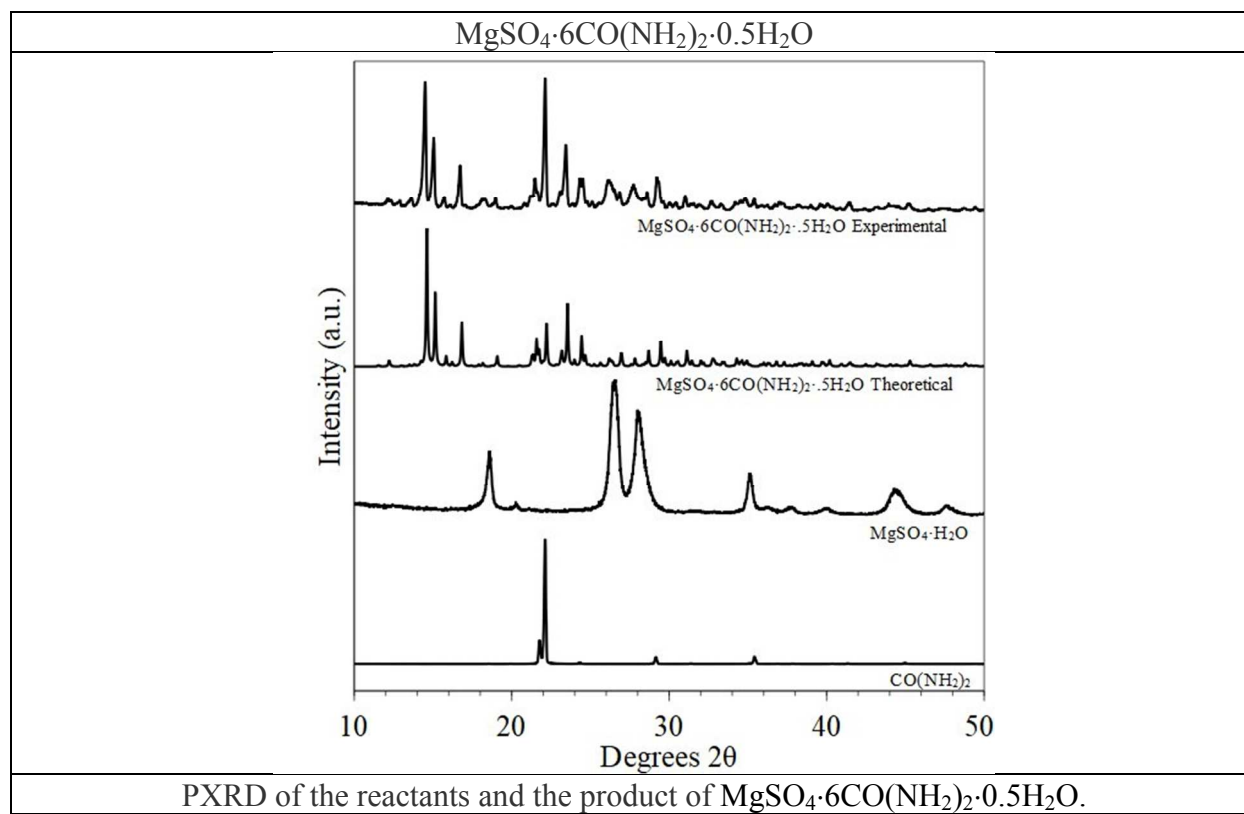
Department of Chemical and Biomolecular Engineering, Lehigh University, B336 Iacocca Hall,  
111 Research Drive, Bethlehem, PA 18015, USA

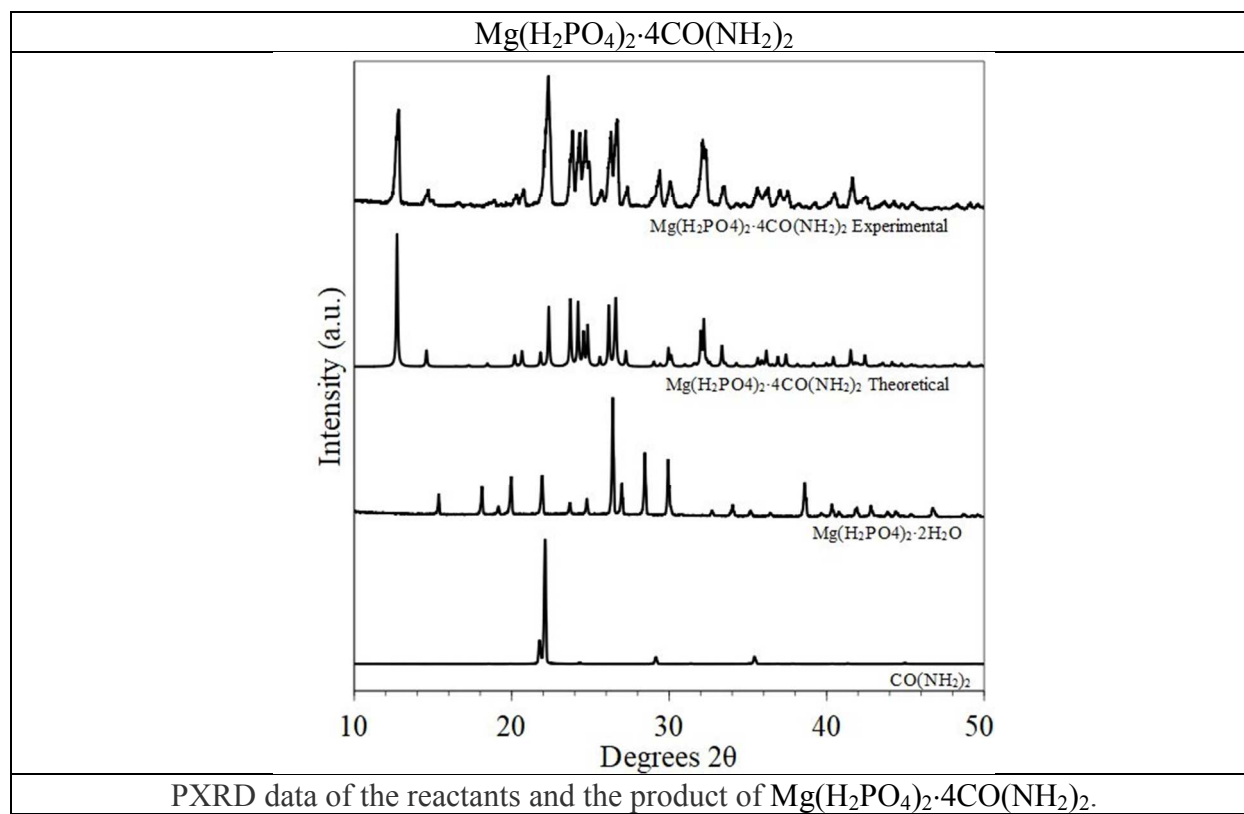
**Figure S1.** Powder XRD patterns of the reactants, urea ionic cocrystals and simulated theoretical. Theoretical XRD patterns were simulated of the crystal structures obtained from Cambridge Crystallographic Data Centre (CCDC).

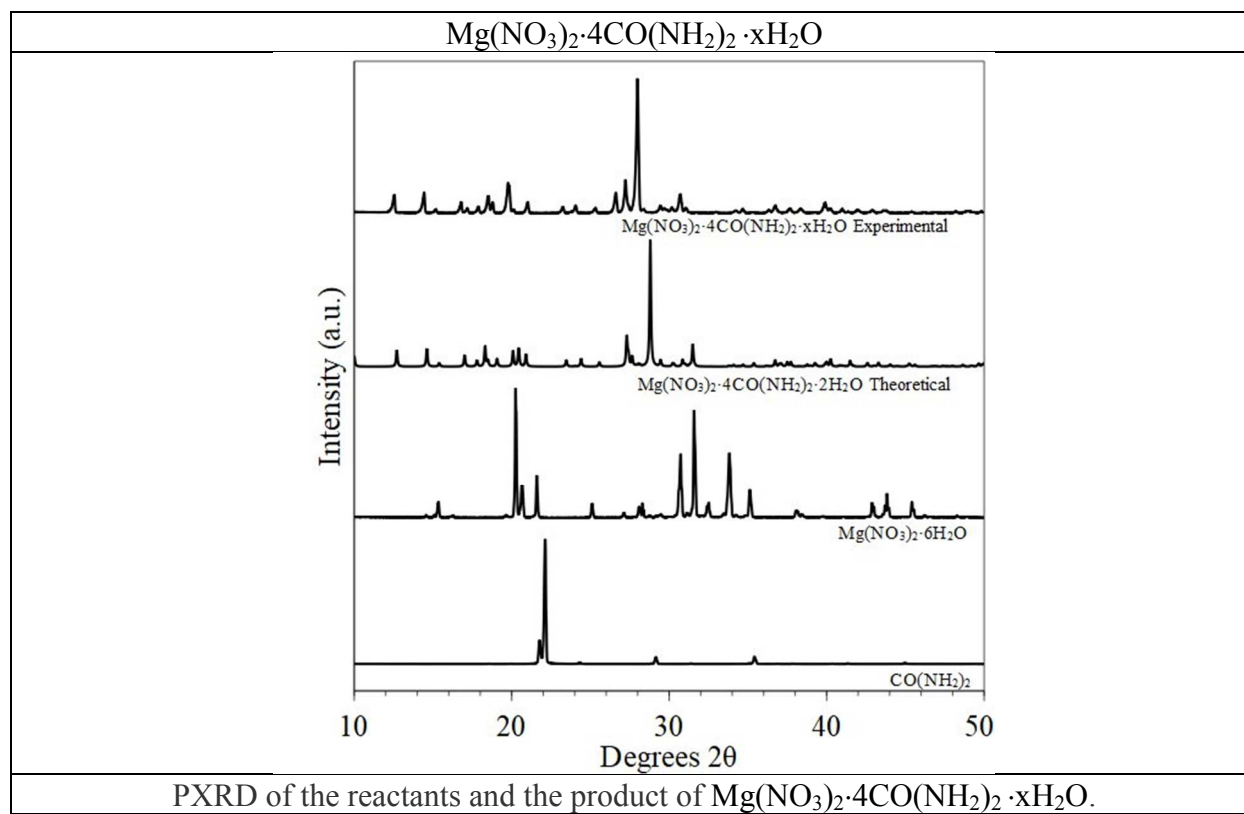


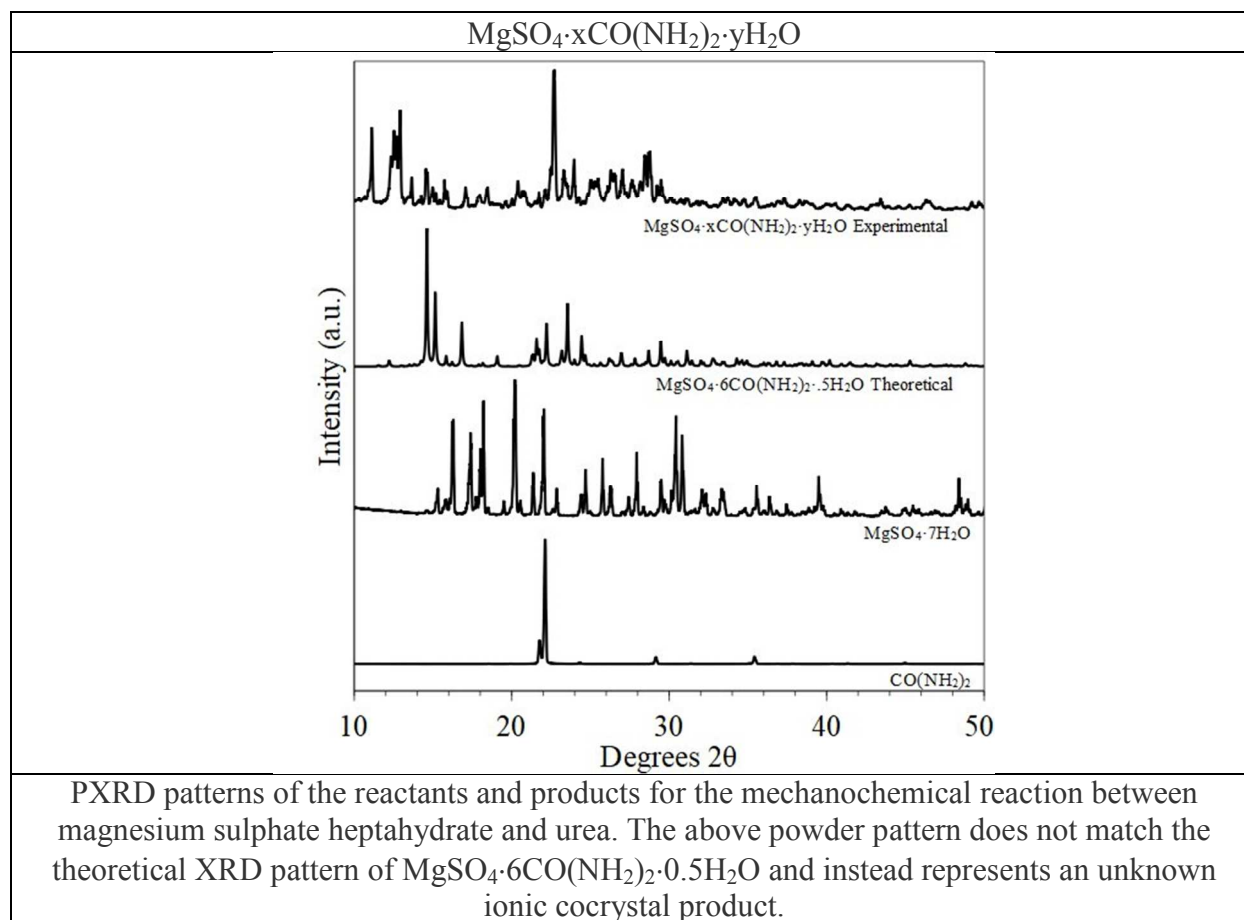












PXRD patterns of the reactants and products for the mechanochemical reaction between magnesium sulphate heptahydrate and urea. The above powder pattern does not match the theoretical XRD pattern of  $\text{MgSO}_4 \cdot 6\text{CO}(\text{NH}_2)_2 \cdot 0.5\text{H}_2\text{O}$  and instead represents an unknown ionic cocrystal product.