A novel dual-action plant fertilizer and urease inhibitor: the urea·catechol co-crystal - characterization and environmental reactivity

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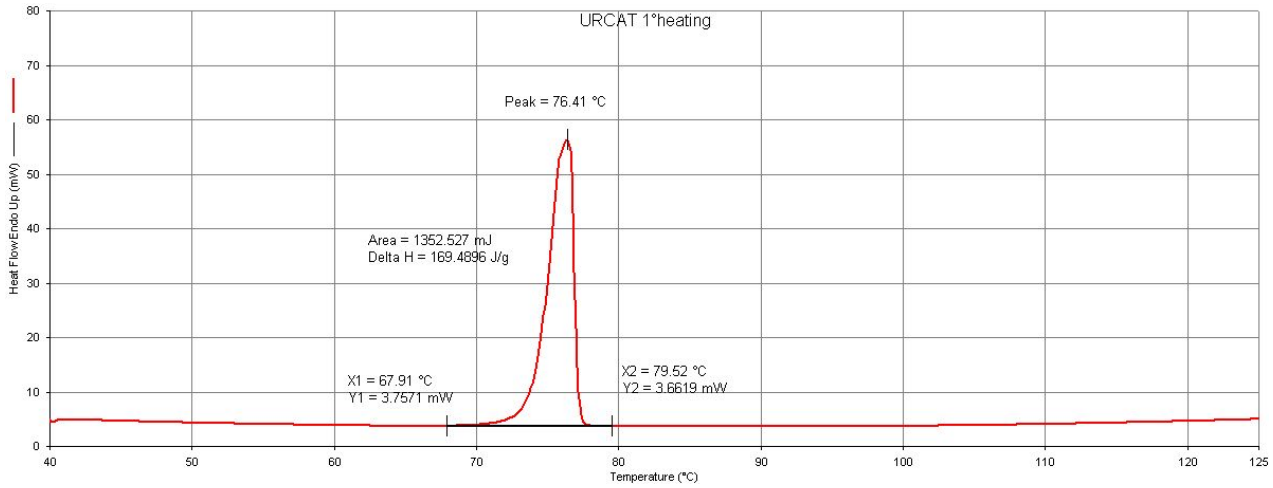

Fig. S1: DSC trace for URCAT (1st heating).

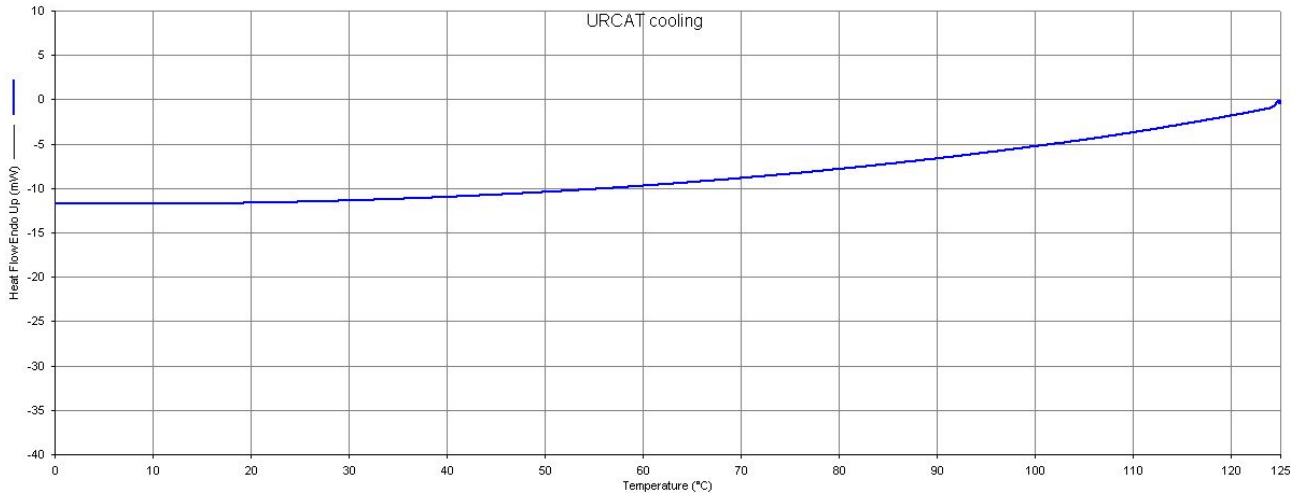

Fig. S2: DSC trace for the urea·catechol co-crystal (URCAT, 1st cooling).

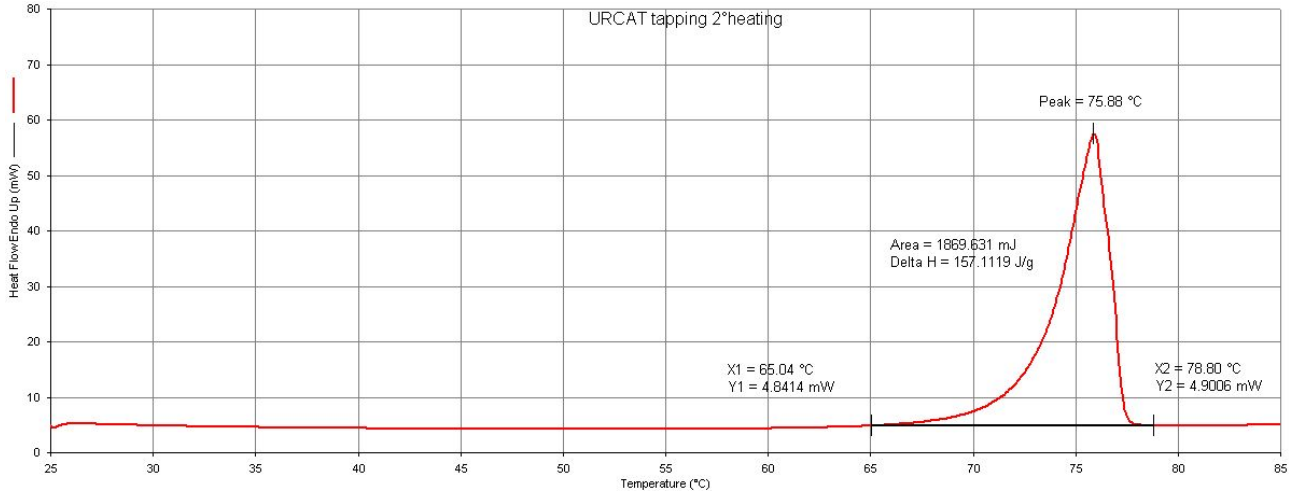

Fig. S3: DSC trace for URCAT (2nd heating). The melting point corresponds to the one observed for URCAT.

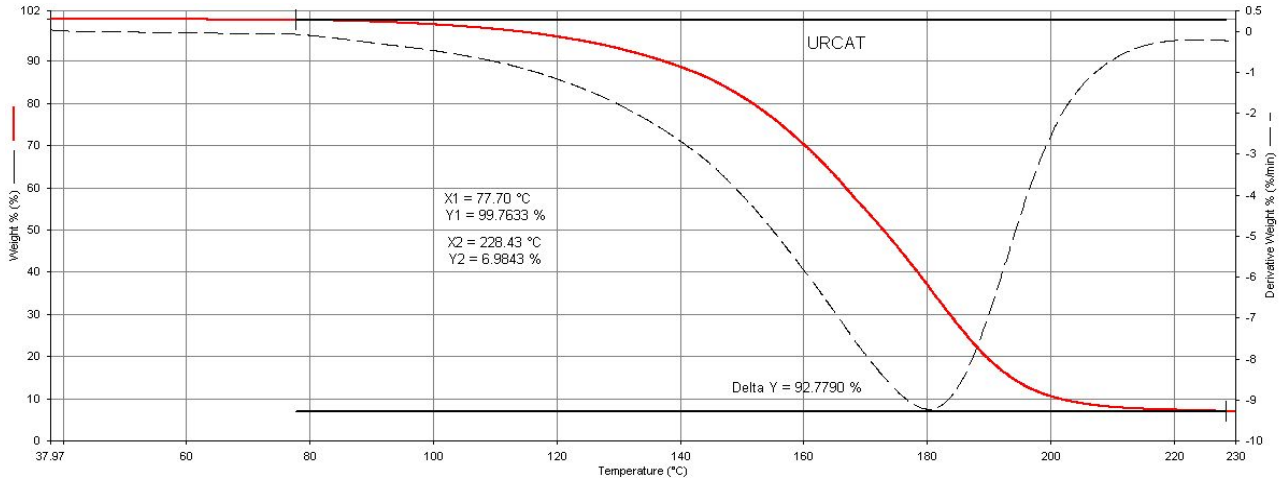

Fig.S4: TGA trace for URCAT.

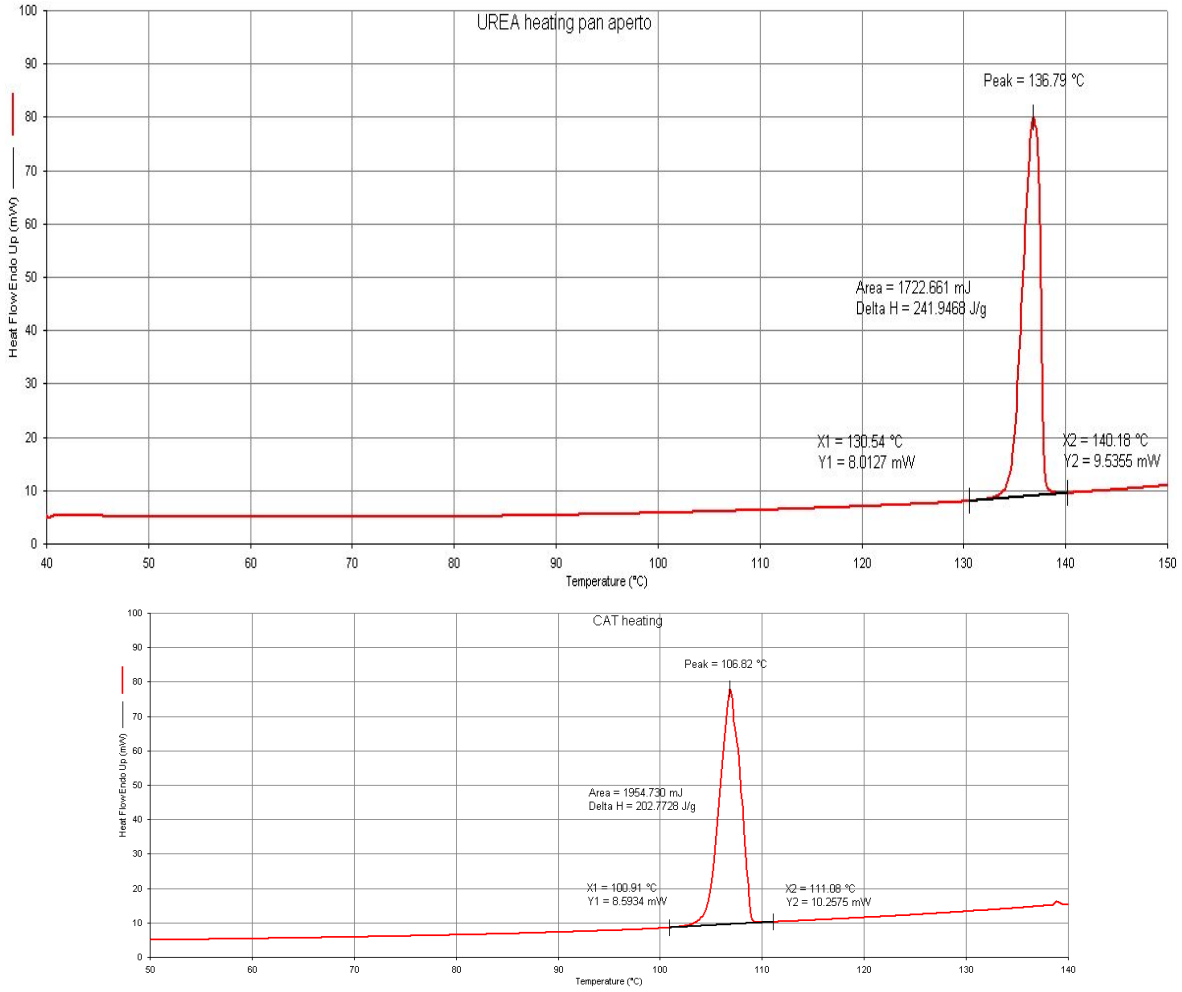

Fig. S5: DSC traces for urea (top) and catechol (bottom) used for the synthesis of URCAT.

Table S1. Crystal data and details of measurement for URCAT.

Chemical formula	$CH_4N_2O \cdot C_6H_6O_2$
M_r, g mol^{-1}	170.17
T / K	293 (2)
Morphology, colour	Plate, colourless
Crystal system	Monoclinic
Space group	$P2_1/c$
a / Å	7.1751 (4)
b / Å	6.2509 (4)
c / Å	19.2212 (16)
α / °	90
β / °	97.888 (7)
γ / °	90
V / Å^3	853.93 (10)
Z	4
d / g cm^{-3}	1.324
μ / mm^{-1}	0.11
Measd reflns	3897
Indep reflns	1976
Reflns with I > 2σ(I)	1255
R_{int}	0.028
R [F^2 > 2σ(F^2)]	0.062
wR (F^2)	0.182

Crystal data can be obtained free of charge from the Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk and have been allocated the accession number CCDC 1880413.