**MS7-P3** **Metformium guanylurea salt of decavanadate, $(HMet^{+})_2(HGU^{+})_4(V_{10}O_{28}^{6-})\cdot 2H_2O$.** Aungkana Chatkon,[ab] Alexa Barres,[b] Kenneth J. Haller,[a] and Debbie C. Crans,[b] [a]*School of Chemistry, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima 30000 Thailand,* [b]*Department of Chemistry, Colorado State University, Fort Collins CO 80523 USA*
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Metformin is an oral antidiabetic drug used in the clinic for treatments, including of malaria, cancer, and Alzheimer's disease [1], [2]. [3], [4]. Metformin is not metabolized in humans and elimination only occurs via the kidneys. The Closed Bottle test (OECD 301 D) shows metformin to be stable in environmental surface waters, but it can be degraded in aerobic bacterial conditions [5]. It is also stable to photolysis and heating at neutral pH, but can be degraded under acid, alkaline, or oxidative conditions [6], [7].

The title compound was obtained after preparation of complexes of two antihyperglycemic agents, metformin and decavanadate, by heating mixed compounds in aqueous solution at pH 6.5 (adjust pH by 1 M NaOH) at 60 °C for 15 hours. The hydrolysis reaction of metformin was investigated using $^{13}C$ NMR spectroscopy, and formation of guanylurea was observed at slightly acidic pH and heating for 20 hours to 70°C. These observations led us to propose that metformin hydrolysed to form guanylurea during the crystallization. The yellow decavanadate product, crystallizes in triclinic *Pî; a* = 10.5330(4); *b* = 10.9952(3); *c* = 12.9375(5) Å; $\alpha$ = 84.7947(15)°; $\beta$ = 67.1390(19)°; $\gamma$ = 87.1139(15)°; *V* = 1374.75 $A^3$; *Z* = 1; $D_{calc}$ = 2.013 Mg $m^{-3}$; $\lambda_{MoK\alpha}$ = 0.71073 Å; $\mu$ = 1.73 $cm^{-1}$; *T* = 100 K; 35924 data collected, $R_{int}$ = 0.0332 for 9070 unique data; $R_1$ = 0.0309 for 6798 $Io > 2\sigma(Io)$; $_{max}$ = 0.39(8). The structures of the ions correspond to those reported previously. The decavanadate anion ($V_{10}O_{28}^{6-}$) lies on an inversion center and charge is balanced by two metformium ($HMet^{+}$) and four guanylurea ($HGU^{+}$) cations. These ions and two waters of solvation engage in an extensive supramolecular hydrogen bonding network with multiple interactions which stabilize the material.

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**MS7-P4** **XRD, Vibrational, and Thermal Characterization of Theophylline: Carboxylic Acid Adducts.** Kenneth J. Haller[a] and Weenawan Somphon[b], [a]*School of Chemistry, Institute of Science, Suranaree University of Technology, Nakhon Ratchasima 30000 Thailand,* [b]*Chemistry Department, Faculty of Liberal Arts and Science, Kasetsart University, Kamphaeng Saen Campus, Nakhon Pathom 73140 Thailand.*
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Theophylline (TP) is an active pharmaceutical ingredient (API) used as a bronchodilator in treatment of respiratory diseases such as asthma. TP is known to exist as a monohydrate and as three anhydrous forms [1], and monohydrate and anhydrous forms can be interconverted as a function of relative humidity (RH). Physicochemical properties of API, including solubility, and humidity, chemical and thermal stability, can be altered (improved) by cocrystallizing the API with another compound. Herein we present the cocrystallization of TP with salicylic acid (SA), 1,3,5-benzenetricarboxylic acid (BTC), and picolinic acid (PI). The 2:1 TP-SA and TP-PI, and the 1:1 TP-BTC were screened by solvent drop-grinding. Crystals were grown by slow evaporation with pH controlled at 2 and 7. Products of TP-SA (2:1) and TP-BTC (1:1) exhibited lower melting points when compared to pure TP. XRD spectra show that new compounds were formed. FT-IR and FT-Raman spectra indicate the nature of the interactions between the two components in the lattices. The (C=O) and (N–H) bands of TP shift lower and higher, respectively, and the (O–H) bands of SA, BTC, and PI shift higher, as compared with the starting materials. All solid cocrystals were stable at room temperature to relative humidity controlled at 59-62% for two weeks. TGA and DSC results will also be presented.

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