

Honors Cup Synthetic Proposal

Section: 220-II

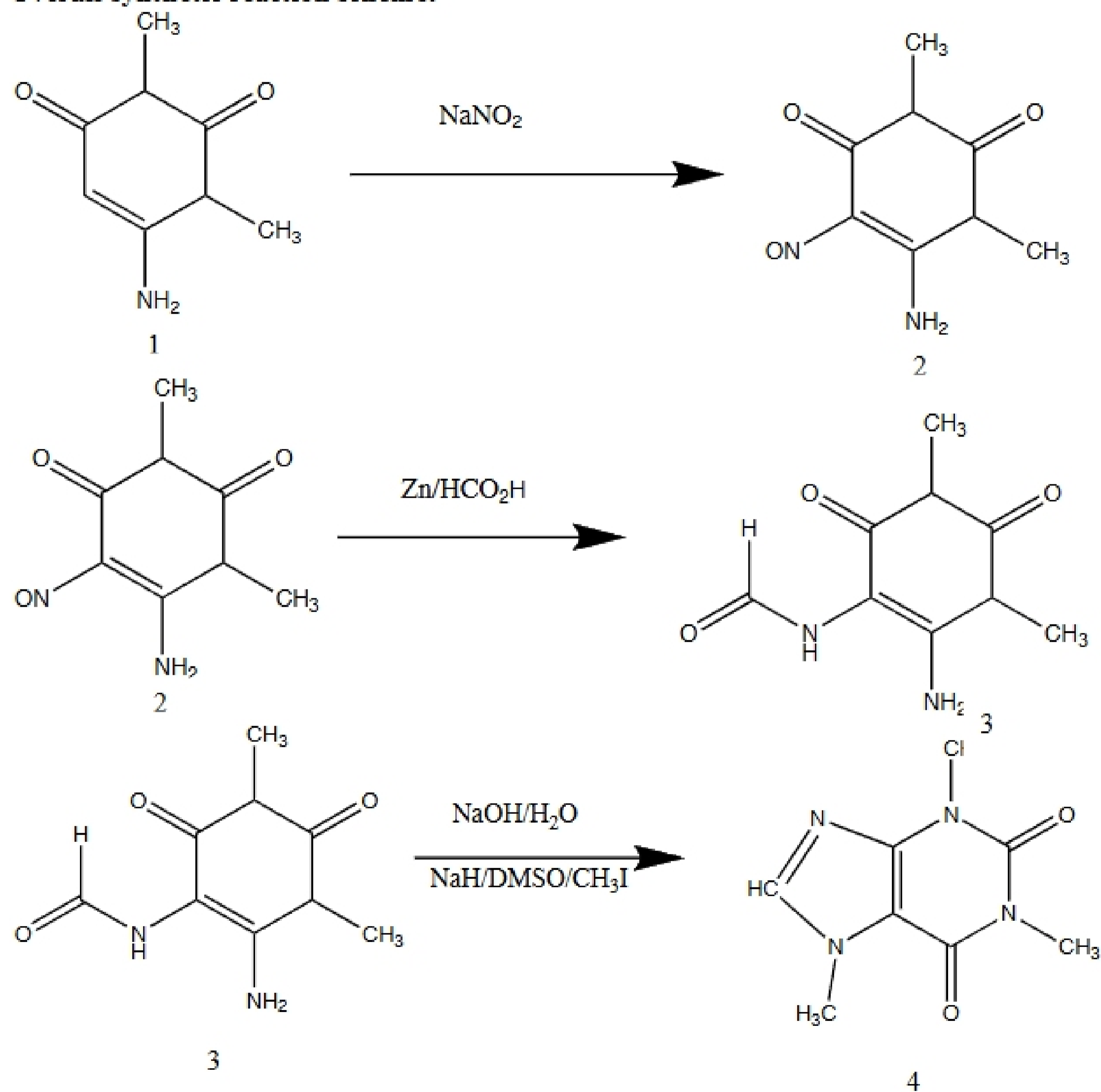
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Title: Synthesis of 1,3,7-trimethyl-1H-purine-2,6(3H,7H)-dione (Caffeine)

Introduction: (what makes your target interesting?)

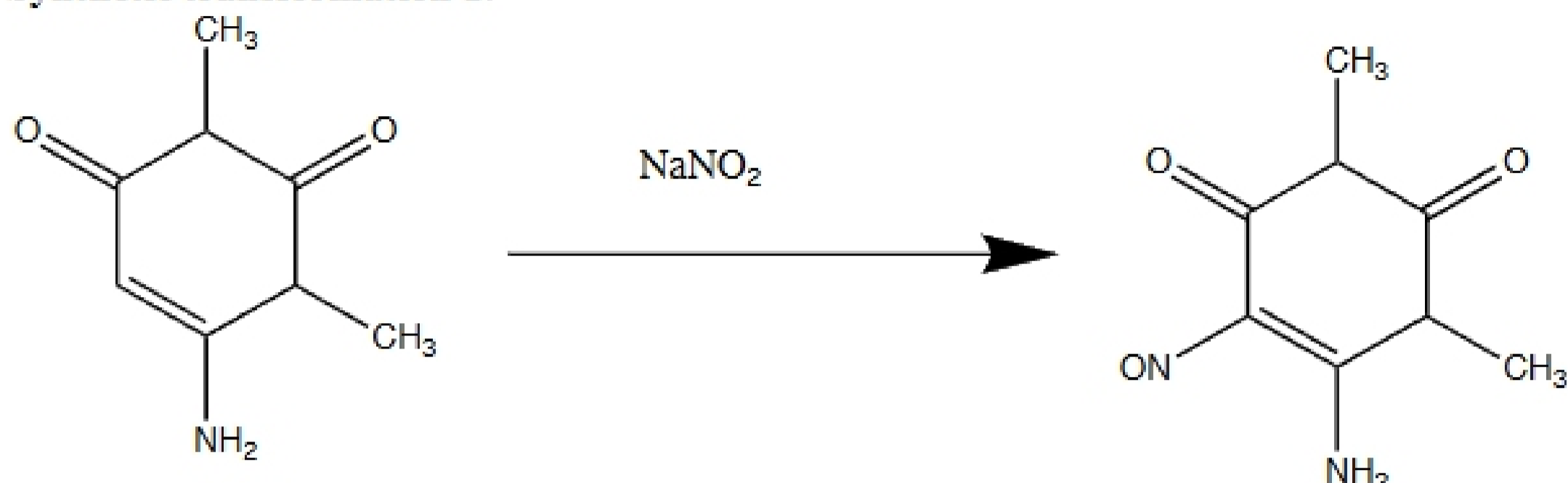
This particular target is interesting because it more commonly referred to as caffeine. Caffeine stimulates the central nervous system causing increased alertness and wakefulness and increased focus. It improves one's general body coordination. The following proposal is the synthesis of caffeine from 6-amino-1,3-dimethyluracil.

Overall synthetic reaction scheme:



Step 1

Synthetic transformation 1:



Experimental 1

A suspension solution of **1** (4.29 mmoles) in water (6.44 ml) was cooled in an ice bath to 0-5°C and then sodium nitrite (4.29 mmoles) in water (1.07 ml) was added. Dropwise addition of acetic acid (12.88 mmoles) with stirring caused nitrosation with a separation of light violet crystals. The resulting precipitate was washed by dimethyl ether and dried in a vacuum dessicator for 24 h to give **2**.

Expected yield: 85 % .665 g

Safety, disposal and green issues 1:

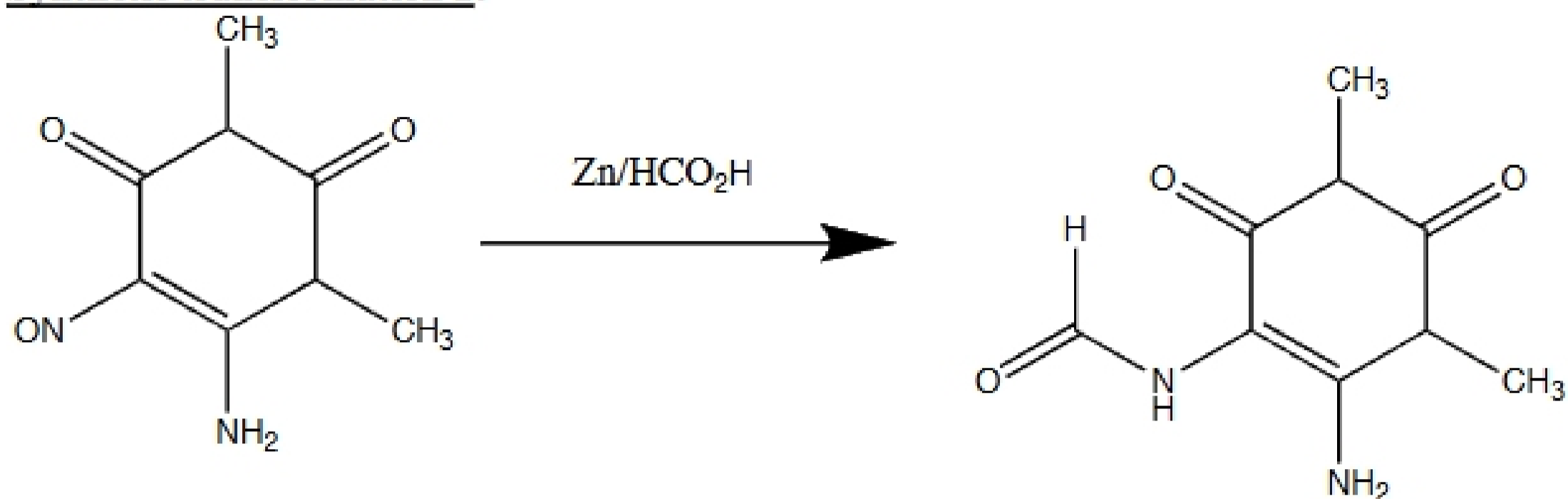
Sodium nitrite- Contact with combustible material may lead to fire. Toxic if swallowed. Severe eye irritant. Respiratory and skin irritant. May act as a carcinogen for chronic exposure.

Acetic acid- Flammable. This material is strongly corrosive and causes serious burns. Very harmful if swallowed.

Ether- Extremely flammable. Harmful by ingestion, inhalation, or through skin contact

Step 2

Synthetic transformation 2:



Experimental 2

Zinc dust (10.95 mmoles) was gradually added to a mixture of 2 (3.65 mmoles) and formic acid (9.2 mL) with stirring. The mixture was heated under reflux for 15 minutes and the excess of zinc and zinc formate were removed by filtration of the hot solution. The filtrate was evaporated under vacuum to dryness. The residue was washed with a little ethanol and recrystallized from water to give 3.

Expected yield: 74% .529 g

Safety, disposal and green issues 2:

Zinc Dust: Flammable, slightly hazardous skin irritant. Keep away from oxidizing agents, alkalis, acids, and moisture.

Zinc Formate: Not hazardous