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We have investigated on the reaction of 2(1H)-pyrimidinones with NaBH_4 . 1-Phenyl-4,6-dimethyl-2(1H)-pyrimidinone (1) reacted with large excess of NaBH_4 in methanol to give three products, 2-oxo-1-phenyl-4,6-dimethyl-1,2,3,6-tetrahydropyrimidine (2), 2-oxo-1-phenyl-4,6-dimethyl-1,2,3,4-tetrahydropyrimidine (3) and 2-oxo-1-phenyl-4,6-dimethyl-1,2,3,4,5,6-hexahydropyrimidine (4). The ratio of three products depends sensitively upon reaction time and reaction conditions. Therefore, we tried the selective preparation of 2-oxotetrahydropyrimidines and 2-oxohexahydropyrimidines.

Pyrimidinone 1 was stirred with NaBH_4 in the presence of trimethyl borate in ethanol to afford compound 2 and trace of compound 3. In the presence of sodium hydroxide, pyrimidinone 1 was treated with NaBH_4 in methanol to give compound 4 and trace of compound 3.

Also, 1-aryl-4,6-dimethyl-2(1H)-pyrimidinones reacted with NaBH_4 in acetic acid to yield only the 2-oxohexahydropyrimidines, while 1-phenyl-2(1H)-pyrimidinone (5) and 1,6-diphenyl-4-methyl-2(1H)-pyrimidinone (6) predominantly gave the corresponding 2-oxotetrahydropyrimidines. The selectivity of this reaction was discussed by UV spectrum, and Force Field and INDO calculations.

We could obtain selectively the 2-oxotetrahydropyrimidines and 2-oxohexahydropyrimidines on the reaction of 2(1H)-pyrimidinones with NaBH_4 under various conditions.

