〔Chem. Pharm. Bull., **33**, 1707 (1985)〕

Synthesis of Some N-Substituted 1, 2, 3, 4, 5, 6-Hexahydro-2, 6-methano-3-benzoazocines (6, 7-Benzomorphans). MIKIO HORI*, EIJI IMAI, NORIHIRO KAWAMURA, TATSUNORI IWAMURA, TADASHI KATAOKA, HIROSHI SHIMIZU

In order to study the effects of N-substituents of benzomorphans on antagonist-agonist activity we synthesized several benzomorphan derivatives having N-alkenyl, alkylnyl, pyranyl or oxetanylmethyl groups. Reduction of N-(hepta-2,5-diyn-4-yl)benzomorphan with Lindlar catalyst resulted in dealkylation to afford normetazocine, whereas reduction with diisobutylaluminum hydride gave N-(hept-2-en-5-yn-4-yl)benzomorphan. N-Dihydro- and tetrahydropyran derivatives were obtained by the reduction of normetazocine with 4-methoxypyrylium salt followed by reduction with sodium borohydride.

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Reactions of 8, 9-Dihydroxanthines with Acetylenic Compounds. Formation of Heteropropellanes MIKIO HORI*, TADASHI KATAOKA, HIROSHI SHIMIZU, EIJI IMAI, YUKIHARU MATSUMOTO

Reactions of 7-substituted 1,3,9-trimethyl-8,9-dihydroxanthines with dimethyl acetylenedicarboxylate afforded heteropropellanes, 7-substituted 4,5-(bismethoxylcarbonyletheno)-1,3,9-trimethyl-4,5,8,9-tetrahydropurine-2,6-diones. The reactions with methyl propiolate afforded pyrimido〔4,5-b〕〔1,4〕diazepine derivatives as well as propellanes when the xanthines have small substituents at *N*-7. When the reaction was conducted in EtOH, 5-{(trans-2-methoxycarbonylvinyl)-methylamino}-6-(ethoxymethylenemethylamino)-1,3-dimethyluracil in 89% yleld. The formation of propellanes was stepwise addition to the 4,5 double bond of xanthine and that of pyrimidodiazepine initiated at the *N*-7 followed by claevage of 8,9-bond and recyclization.

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New Description of the Substituent Effect on Electronic Spectra by Means of Substituent Constants. III. Charge Transfer Spectra of EDA Complexes. TANEKAZU KUBOTA*, BUNJI UNO, KENJI KANO, YŌICHI NINOMIYA

General equations in order to describe the electronic spectra by means of substituent constants were derived on the basis of molecular orbital theory. The most suitable substituent constants are theoretically Swain's F and R constants, but Yukawa-Tsuno's parameter is also useful for π-electron system. In this paper these equations were applied to explain the charge transfer spectra of π-π type EDA complexes composed of TCNE and various kinds of aromatic donors. The results have been quite reasonable and discussed in detail.