# *Synthesis of a Pseudo-Cross-Conjugated Heterocyclic Mesomeric Betaine (PCCMB)*

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**Abstract:** Treatment of N,5,6-trimethyl benzimidazole with (chlorocarbonyl)phenyl ketene (I) afforded anhydro-1-hydroxy-3-oxo-2-phenyl-5,6,8-trimethylpyrrolo[2,1-b] benzimidazolium hydroxide.

**Introduction**

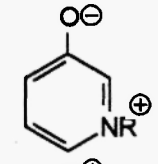
We have recently reported on the cycloaddition reaction of (chlorocarbonyl)phenyl ketene (I) with carbonyl compounds (1) and C=N linkages (2, 3). Reaction of (II) with several oximes resulted in a series of cross-conjugated heterocyclic mesomeric betaines CCMB (4).

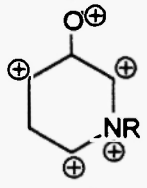
A pseudo-cross-conjugated heterocyclic mesomeric betaine PCCMB was prepared from 1-substituted benzoimidazole and (chlorocarbonyl)phenyl ketene (II) at ambient temperature. This synthesis requiers the generation of reactive intermediate capable of forming both C-C and C-N union bond from a CH=N group and 1.3-bielectrophile (5).

**Results and discustions**

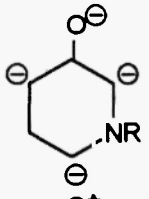
The classification of conjugated heterocyclic mesomeric betaines, the cross-conjugated heterocyclic mesomeric betaines and the pseudo-cross-conjugated heterocyclic mesomeric betaines are as followes.

## Conjugated Heterocyclic Mesomeric Betaines

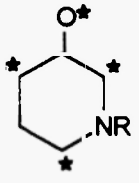




possible sites for positive charges

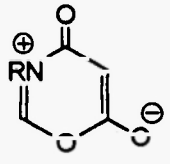


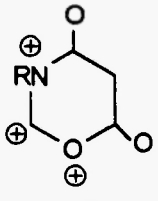
possible sites for negative charges



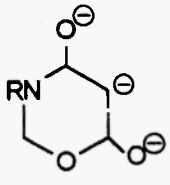
common sites for positive and negative charges

## Cross–Conjugated Heterocyclic Mesomeric Betaines (CCMB)

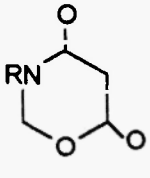




possible sites for positive charges

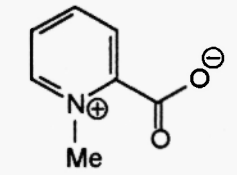


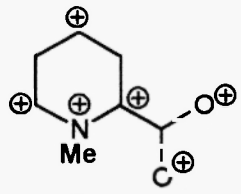
possible sites for negative charges



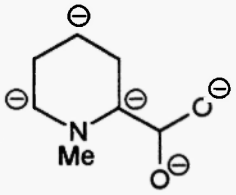
common sites for positive and negative charges

**Pseudo—Cross— Conjugated Heterocyclic Mesomeric Betaines (PCCMB)**

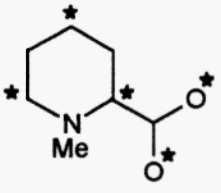




possible sites for positive charges



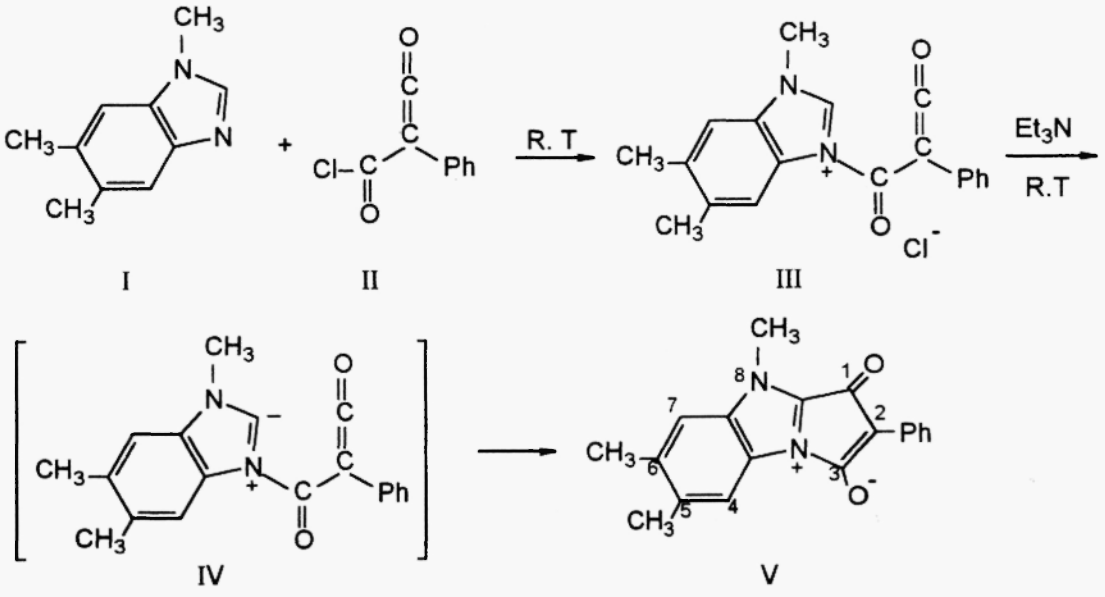
possible sites for negative charges



common sites for positive and negative charges

"*The dipolar canonical forms associated with pseudo-cross-conjugated heterocyclic mesomeric betaines (PCCMB) include not only electron octet formulate and electron sextet formulate associated with internal electron octet stabilization, but also electron sextet formulate without internal electron octet stabilization*" *(6).*

Thus equimolar quantities of N,5,6-trimethyl benzimidazole and (II) readily underwent reaction in the presence of triethylamine in dry ether giving anhydro-1-hydroxy-3-oxo-2-phenyl-5,6,8-trimethylpyrrolo[2,1-b]benzimidazolium hydroxide in 62% yield with a mp of 160C. A yellow color characteristic of such a compounds developed in the reaction medium. The IR spectrum revealed a band at 1720 $cm^{1}$. The $^{1}$HNMR spectrum of this compound is very simple. It revealed a multiplet at 7.2-8.3 ppm (phenyl protons) and a singlet at 4.3 ppm due to the methyl group attached to the nitrogen and a singlet at 2.4 ppm due to methyl groups attached to the benzene ring. The $^{13}$CNMR spectrum is consistent with the structure V.




**Acknowledgment**

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**References**

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6. An excellent review article was published by professor W. D. Ollis and his colleagues entitled "Heterocyclic Mesomeric Betaines", see the following reference.
   W. D. Ollis, S. P. Stanforth and C. A. Ramsden, *Tetrahedron.*, **41**, 2239, (1985).

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