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Structuw-Reactivity Correlation of Phosphonyl Transfer Reactions of Wines with Diphosphonate; Ab Initio Mo and Experimental Studies

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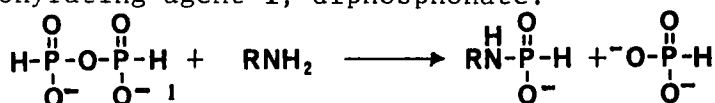
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Y. BABA

The present author investigated the structure-reactivity correlation in the reactions of amines with P-O-P bridged phosphorylating agent **1**, diphosphonate.



The rate constants determined by following the rate of disappearance of 1, for the reactions in an aqueous solution at 30 °C and ionic strength 1.0, are plotted logarithmically against the basicities of the amines in Fig. 1. The plot shows good linearity with β -value of 0.52. Using ab initio computations, the author have also determined the free energies of the reactions. The relationship between computed free energies and basicities of the amines in the gas phase or observed rate constants was discussed. The results are consistent with a concerted reaction mechanism with a single, symmetrical transition state.

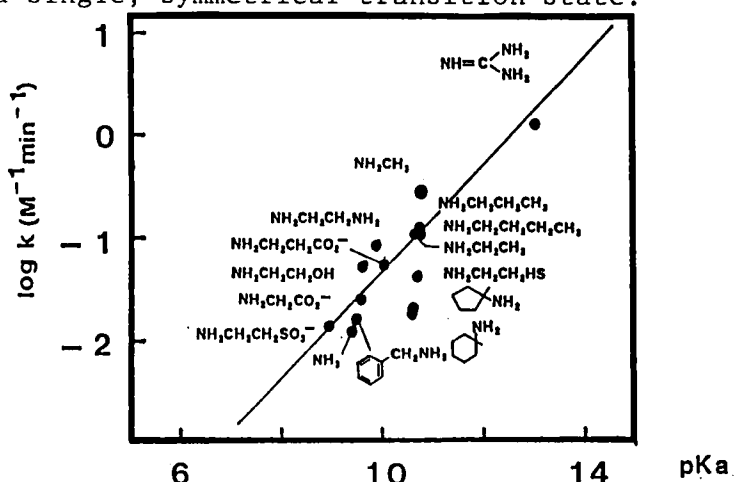


Fig. 1 Brønsted-type plot for the reaction of 1 with amines. The pK_a and k are statistically corrected.