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CLASSIFICATION OF SUBSTITUENTS IN PHOSPHORUS COMPOUNDS BY PATTERN RECOGNITION

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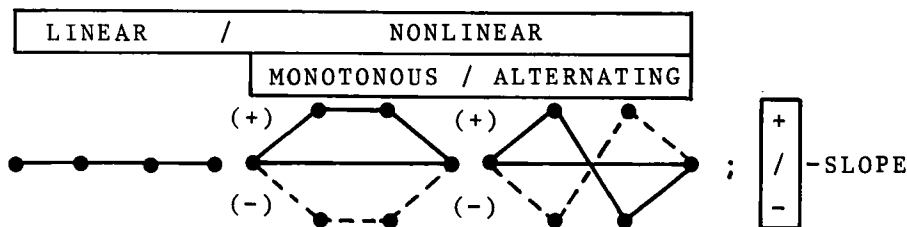
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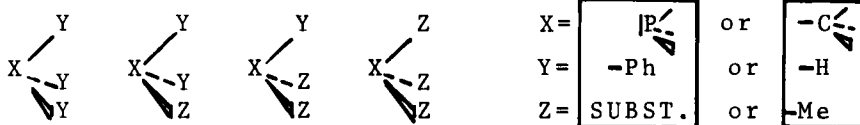
Abstract The importance of pattern recognition to identify factors mediating order in chemistry will be demonstrated.

INTRODUCTION

Complex chemical systems with overwhelming covalent interactions will normally not show linear dependencies or additivity rules for factors (parameters) mediating order like in cis-/trans-, R-/S- or ortho-/para- isomer formation. The simplest procedure to elucidate increasing linear, nonlinear monotonous or alternating behavior (ten different patterns)



e.g. is a systematic variation (ODD/EVEN or EVEN/ODD) at tetrahedral centers from 3,2,1 to 0 or 0,1,2 to 3:



EXAMPLES AND RESULTS

By substituting phenylgroups in triphenylphosphane by substituents with central atoms of 4th or 6th group of PSE Tolman's additivity rule¹⁾ is not fulfilled²⁾. By a meta-pattern (a pattern of patterns) the general order factors ODD/EVEN, S/AS and DO/ACC (relative to carbon) become evident. Triphenylphosphane is a natural standard ($P_{\text{TPP}} = 3 P_{\text{Ph}} = 0$; equally populated left/right propeller arrangements).

In chemical systems absolute and relative control of 4q-/4q+2-, cis-/trans- or R-/S- order in products is demonstrated^{3,4)} by representative substituents like -R/-OR (S/AS or AS/S) and -SMe/-OMe or -CMe₃/-SiMe₃ (DO/ACC). Pattern recognition is extremely helpful especially in relative control of order. Compensation phenomena may destroy important information. But compensation phenomena - introduced by will - are necessary to provoke complementarity. Hereby an inverse optical induction is mediated by order factors of achiral subsystems.

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