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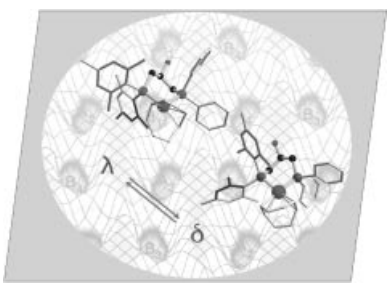
COVER PICTURE

The cover picture shows two conformations of the chiral chelate cation $[\{\kappa\text{-P(Mes)}_2\text{CH}_2\text{CH(OH)CH}_2\text{-}\kappa\text{-P(Ph}_2\}\text{Rh}(\eta^4\text{-COD})]^+$ which is active as an enantioselective hydrogenation catalyst. The δ- and λ-twist conformations of the six-membered diphosphane chelate cycle are shown together with a projection of the hypersurface relevant to the transition between these enantiomeric forms. The hypersurface is generated by force field calculations. The specific force field is derived by refinement of the relevant force field parameters by genetic algorithms on the basis of eleven compounds of this type. The predictions made by this model are in almost quantitative agreement with the experimental data: The λ-form is calculated to be 3.1 kJ•mol^{-1} more stable than the δ-form (experimental: 3.4 kJ•mol^{-1}). The δ ⇔ λ transition is predicted to be accompanied by a coupled rotation of the mesityl groups (color code in the cover picture) in full agreement with the experimental results. The upper threshold of the activation barrier of the transition is calculated to be 69.1 kJ•mol^{-1}; the experimental value is 64.4•kJ mol^{-1}. This novel approach to molecular modeling is described in the article by G. Huttner et al. on p. 3111 ff. The quantitative NMR analysis of the structure and dynamics of compounds containing six-membered diphosphane chelate cycles is presented in the accompanying article by G. Huttner et al. on p. 3129 ff.



MICROREVIEW

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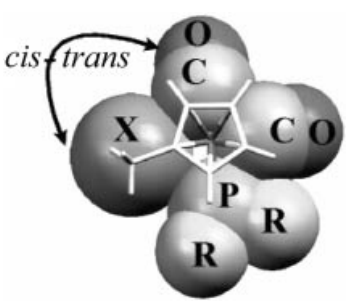

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