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Benzoxaboralone: A Boronic Acid with High Oxidative Stability and Utility in Biological Contexts

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Abstract : The presence of a nearly vacant p orbital on boron endows boronic acids with unique abilities as a catalyst and ligand. An organocatalytic process has been developed for the conversion of biomass-derived sugars to 5-hydroxymethylfurfural, which is a platform chemical. Specifically, 2-carboxyphenylboronic acid (2-CPBA) has been shown to be an optimal catalyst for this process, promoting the desired transformation in the absence of metals. The attributes of 2-CPBA as a catalyst led to additional investigations of its structure and reactivity. 2-CPBA was found to exist as a cyclized benzoxaborolone adduct rather than a free carboxylic acid. This cyclization has profound consequences for the oxidative stability of the boronic acid. Stereoelectronic effects within the oxaborolone ring destabilize the oxidation transition state by reducing electron donation from the cyclic oxygen to the developing p orbital on boron. That leads to a 10,000-fold increase in oxidative stability while maintaining the normal reactivity of boronic acids toward diols (e.g., carbohydrates) and nucleophiles in proteins while also presenting numerous hydrogen-bond accepting and donating groups. Thus, benzoxaborolones are useful in catalysis, chemical biology, medicinal chemistry, and allied fields.

Keywords : bioisosteres, boronic acid, catalysis, oxidative stability, pharmacophore, stereoelectronic effects
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