

# Quantum-Chemical and Correlation Study of the Tautomerism and Ionization of 1,2,3-Trihydroxy-9,10-anthraquinone

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**Abstract**—1,2,3-Trihydroxy-9,10-anthraquinone (anthragallol) exists as an equilibrium mixture of the 9,10-, 2,9-, 1,2-, and 2,3-quinoid tautomers. Its anion was detected in the 9,10-, 1,10-, 2,9-, and 2,3-quinoid forms, and its metal complexes, the 9,10- and 2,9-quinoid forms. Ionization and complexation of anthragallol can shift the tautomeric equilibrium.

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