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equilibrium geometry

Molecular geometry that corresponds to the true minimum on the respective potential energy surface. While information relating to the equilibrium geometry is provided by calculations within the adiabatic approximation (minimization of the total energy with respect to any independent geometrical parameter), various experiments yield some effective geometries for the molecule which are averaged over molecular vibrations.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1938

