energy gradient

First derivatives of the total energy with respect to nuclear coordinates, \textit{i.e.}, negative values of forces on the nuclei. Evaluation of energy gradient plays a central role in searching potential energy surfaces for stationary points. A widespread technique is based on the minimization of the gradient norm (the square of energy gradient).

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