energy gradient

First derivatives of the total energy with respect to nuclear coordinates, *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).

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