## quantum mechanics/molecular mechanics

Acronym: QM/MM

Also contains definition of: QC/MM

Hybrid procedure for the treatment of large molecular systems. A crucial part of the system (e.g., the chromophore and its surroundings) is treated explicitly by quantum mechanical (QM) techniques, whereas the rest of the system is approximated by a classical or molecular mechanics (MM) force field treatment.

Note:

Sometimes called QC/MM.

## Source:

PAC, 2007, 79, 293 (Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006)) on page 406