

## **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