

**transition (dipole) moment,  $M_{nm}$** 

An oscillating electric or magnetic moment can be induced in an atom or molecular entity by an electromagnetic wave. Its interaction with the electromagnetic field is resonant if the frequency of the latter corresponds to the energy difference between the initial and final states of a transition ( $\Delta E = h\nu$ ). The amplitude of this moment is referred to as the transition moment. It can be calculated from an integral taken over the product of the wavefunctions of the initial ( $m$ ) and final ( $n$ ) states of a spectral transition and the appropriate dipole moment operator ( $\vec{D}$ ) of the electromagnetic radiation:

$$M_{nm} = e \int \Psi_n^* \sum_i Z_i \vec{r}_i \Psi_m \, d\tau$$

where the summation is over the coordinates of all charged particles (electrons and nuclei). Its sign is arbitrary, its direction in the molecular framework defines the direction of transition polarization, and its square determines the strength of the transition. If  $e$  is omitted one obtains  $R_{nm}$  in the sense used in oscillator strength. The SI unit of the transition dipole moment is C m. The common unit is debye (D).

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