

## Glossary of terms in the Crystal Violet Quantum Theory documents

<b>alkaline</b>	Aqueous solution with $\text{pH} > 7$ , where $[\text{OH}^-]$ is greater than $[\text{H}_3\text{O}^+]$
<b>basis set</b>	The collection of atomic orbital functions, such as s, p, or d, on all atoms that are combined to form the molecular orbital functions ( $\Psi$ ) of the molecule.
<b>bleaching</b>	A chemical reaction resulting in the reactant molecule's loss of color.
<b>electrostatic potential</b>	Force that an electron "feels" at a given position near a molecule, which results from the combination of attraction to nuclei and repulsion from nearby electron clouds.
<b>HOMO</b>	Highest Occupied Molecular Orbital. MO with highest energy content that contains 1 or 2 electrons.
<b>hydroxide</b>	$\text{OH}^-$ ion
<b>infrared</b>	Electromagnetic radiation with wavelengths between 750 and 1000 nm. Radiant heat given off by a hot object.
<b>isosurface</b>	Surface around a molecule where a parameter, such as electron density, has all equal values.
<b>lambda max (<math>\lambda_{\text{max}}</math>)</b>	Wavelength of maximum absorption of UV or visible light.
<b>lobe (of MO)</b>	A region of a molecular orbital ( $\Psi$ ) where its value is much greater than, or less than, zero. Analogous to the peak or trough of a sine wave.
<b>LUMO</b>	Lowest Unoccupied Molecular Orbital. MO containing zero electrons, whose energy level is just above the HOMO.
<b>microwave</b>	Electromagnetic radiation with wavelengths between 2 and 1000 mm.
<b>multiplicity</b>	In a molecule, the number of possible spin states ( $m$ ) due to one or more unpaired electrons ( $n$ ): $m = n + 1$
<b>nanometer (nm)</b>	$10^{-9}$ meter
<b>occupancy</b>	How many electrons inhabit an orbital, which can be 0, 1 or 2.
<b>pigment</b>	A color-producing molecule.
<b>radio wave</b>	Electromagnetic radiation with wavelengths between 1 inch and 100 miles.
<b>resonance</b>	Bonding in a molecule where one Lewis formula does not correctly describe the structure, but the best description is a hybrid of 2 or more formulas. Often this is due to a multi-atom $\pi$ -bond such as the one in formate ion.
<b>single point energy</b>	Quantum energy calculation based on a single molecular geometry.
<b>spectrophotometer</b>	An instrument to measure light intensity at a certain wavelength, comparing the intensity going into a sample with the (lower) intensity exiting the opposite side.
<b>triarylmethane dye</b>	Carbon cation (+) carrying three aromatic substituents, such as the dimethylamino phenyl groups in crystal violet.
<b>ultraviolet</b>	Electromagnetic radiation with wavelengths between 100 and 350 nm.
<b>visible</b>	Electromagnetic radiation with wavelengths between 350 and 750 nm.

The following are defined in the Glossary of Burdge and Overby, 4<sup>th</sup> Ed.

**absorbance**

**absorption**

**activation energy**

**alcohol**

**Angstrom**

**aromatic**

**atomic orbital**

**cation**

**dipole moment**

**electron**

**electronegativity**

**electrophilic**

**endothermic**

**exothermic**

**formal charge**

**frequency**

**hydrogen bonding**

**ion**

**Joule**

**kilocalorie (kcal)**

**kinetic energy**

**Lewis formula**

**lone pair**

**molecular orbital**

**molecule**

**nucleus, nuclei**

**pH**

**photon**

**pi-bond ( $\pi$ -bond)**

**p-orbital**

**significant figure**

**thermal energy**

**transition state**

**transmit**

**x-ray**