RhoRix

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Abstracting the Topology

The electron density of a chemical system is a scalar function, mapping points in 3-dimensional real space to a scalar. It is typically written $\rho(\vec{r})$, where $\vec{r} \in \mathbb{R}^3$ is a 3-dimensional vector quantity with real elements. The topology of the electron density consists of series of objects that collect one or more of these vectors into sets based on their shared properties, along with other relevant information. A number of chemical concepts can be discussed in terms of properties defined at any point $\vec{r}$. As such a point can carry additional information. As such we define a Point object as follows: A point consists of a vector, $\vec{r}$, and a set of properties computed at that point. In order to keep the points generic, a dictionary data structure is used for properties that maps a String value to the corresponding stored property, for example the key "ElectronDensity" maps to the real value of $\rho(\vec{r})$. In this manner any property can be included with points, for example at critical points or along an atomic interaction line.

The first topological object to be discussed is the critical point. As the name suggests, this is a single point in space described by a single position vector. It is often differentiated from other points with the notation $\vec{r}_{CP}$. The critical point is defined in terms of the gradient of the electron density, $\nabla\rho(\vec{r})$, which is itself a vector quantity. Critical points are stationary points of the electron density (i.e. $\vec{r}$ where $\nabla\rho(\vec{r}) = 0$. Critical points all share this property, yet they can differ in nature, representing minima, maxima and saddle points of $\rho\vec{r}$. Critical points are further categorised on the basis of $\nabla^2\rho(\vec{r_{CP}})$. The 2nd derivative operator produces a symmetric $3x3$ matrix of values which can be diagonalized to yield 3 eigenvalues. The number of non-zero eigenvalues is the rank ($\omega \in \{1,2,3\}$) of a given critical point, and the sum of their signs is the signature ($\sigma \in \{-3,-2...3\}$). These two integer values serve to completely characterize a critical point and are typically written (ω,σ). The majority of observed critical points are $\omega = 3$ critical points. Critical points of type $(3,-3)$ are maxima, and one such critical point practically coincides with each nucleus in a system. Type $(3,-1)$ critical points appear between atoms and are referred to as bond critical points. Ring critical points are $(3,1)$ and cage critical points are $(3,3)$. Thus a CP object is the

vector $\vec{r_{CP}}$ and the values of (ω, σ).

The remaining topological objects involve sets of points. The most common shared object is the gradient path. This is a line of steepest ascent through the electron density. These are not typically represented analytically, but are located by numerical procedures. As such, their natural representation is as an ordered set of connected points. These lines always begin and end (noting that the direction is not rigorously defined) at either a critical point or at an infinite distance from a critical point. We define a gradient path as an ordered set of points, each connected to the previous, where at each point... Gradient paths can be formed into sets just as points can.

These 'topological objects' are to be rendered for viewing by RhoRix. To achieve this, each particular object must be mapped to a 3-dimensional object that can be drawn.