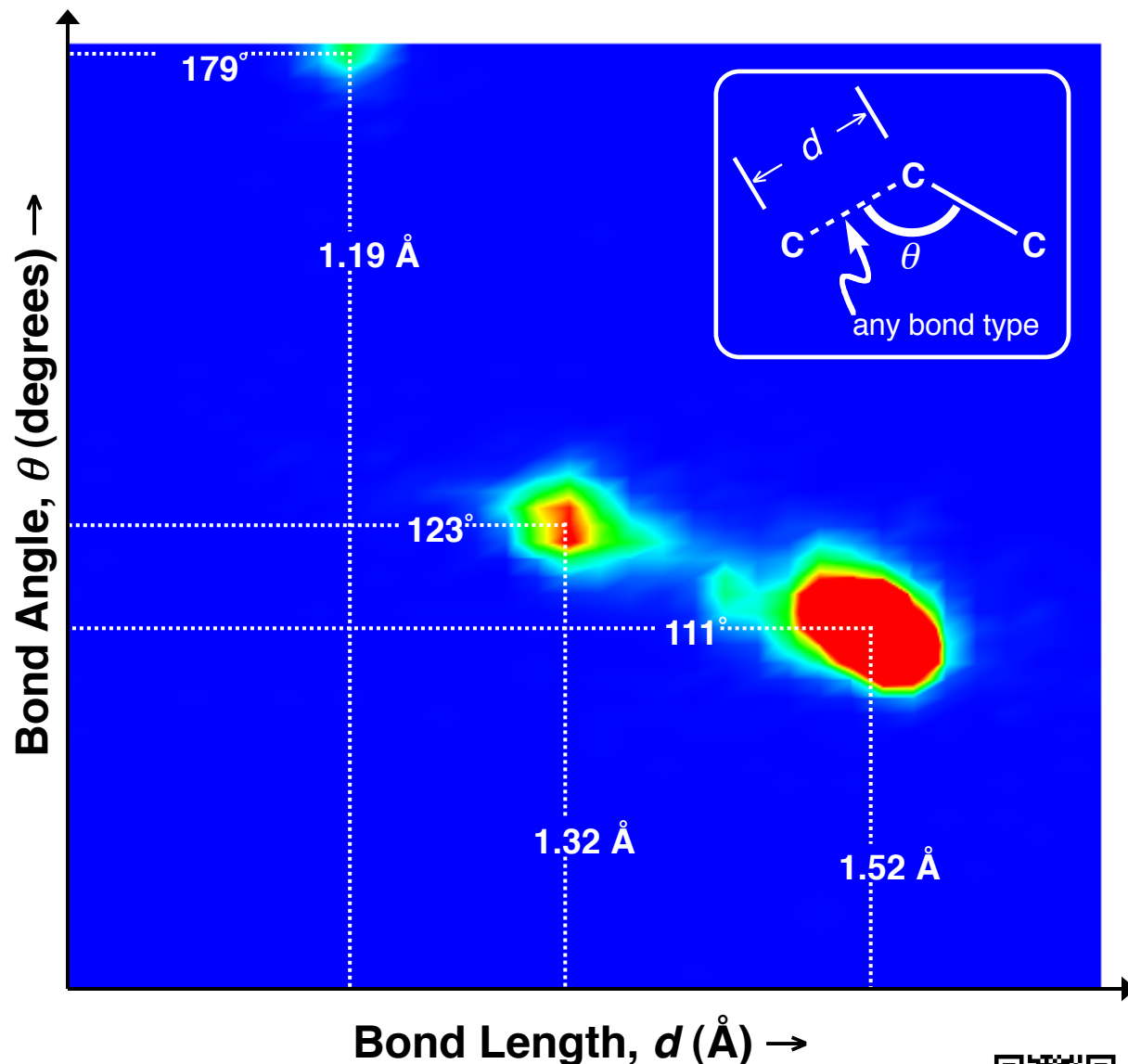


# Validation of the VSEPR Model

Validation of VSEPR – at least as an approximate model for carbon-containing structural fragments – comes from the large collection of structural data that's available in the Cambridge Structural Database. This plot is based on more than 46,000 structural fragments whose geometry has been experimentally determined by X-ray diffraction. Think of this plot like a histogram, whereby each structural fragment is grouped according to its **bond length** and **bond angle** (see the inset for the definition of these parameters). The frequency of occurrence at a particular bond-length and bond-angle is color-coded, red being most frequent, blue being the least. **The plot shows that nearly all of the 46,000 fragments fall within one of three regions.** These regions correspond to **linear** geometry (bond angle ca. 180°), **trigonal planar** geometry (bond angle ca. 120°) and **tetrahedral** geometry (bond angle ca. 110°). The data show a strong correlation between bond length and bond angle. The bond angles are seen to deviate slightly from the ideal angles predicted by the VSEPR model.



# Geometry, Hybridization and Number of EPDs

The valence-shell electron-pair repulsion (**VSEPR**) model predicts an atom's geometry based on the number of electron-pair domains that are present. The VSEPR model states that **the best arrangement of electron-pair domains about an atom is that geometry which maximizes their separation**. Besides predicting geometry, the number of electron-pair domains also determines the atom's state of hybridization.

| geometry or hybridization | number of EPDs |       |     |
|---------------------------|----------------|-------|-----|
|                           | four           | three | two |
|                           |                |       |     |
| Geometry                  |                |       |     |
| Hybridization             |                |       |     |
| AO Combination            |                |       |     |
| % S Character             |                |       |     |