1. For five coordinate compounds, one can define a parameter - Take the two largest valence (LML) angles in the compounds, such that :

This value indicates if we are dealing with a square bipyramid (), a triangular bipyramid (), or something in between, closer to one or the other.

|  |  |  |  |
| --- | --- | --- | --- |
| Square pyramidal geometry | Square pyramidal geometry | Trigonal bipyramidal geometry | Trigonal bipyramidal geometry |

For four coordinated compounds, the best parameter is

In this expression are the two greatest valence angles of the coordination centre, and the interpretation is quite similar to the above one.

|  |  |  |
| --- | --- | --- |
| Square planar geometry | Seesaw geometry | Tetrahedral geometry |
| Square planar geometry | Seesaw geometry | Tetrahedral geometry |

For six coordinated compounds, the most frequent, there is no way to "quantify" the geometry. So, I came up with a

where and are the largest angles in the geometry and is , which is one of the LML angles in the triangular prism. This gives the following values:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | Octa | PBeqa | PBaxa | TriPa |
| d) | 180 | 180 | 144 | 135.585b) |
| d) | 180 | 144 | 144 | 135.585 |
|  | 0 | 0.4053 | 0.8105 | 1 |
|  |  |  |  |  |

Where the middle two geometries are pentagonal bipyramids, one missing an equatorial L atom and the other missing an axial L atom. I'm assuming that these 2 structures can be taken as midpoints in a transition from octahedral to trigonal prism by moving the atoms around.