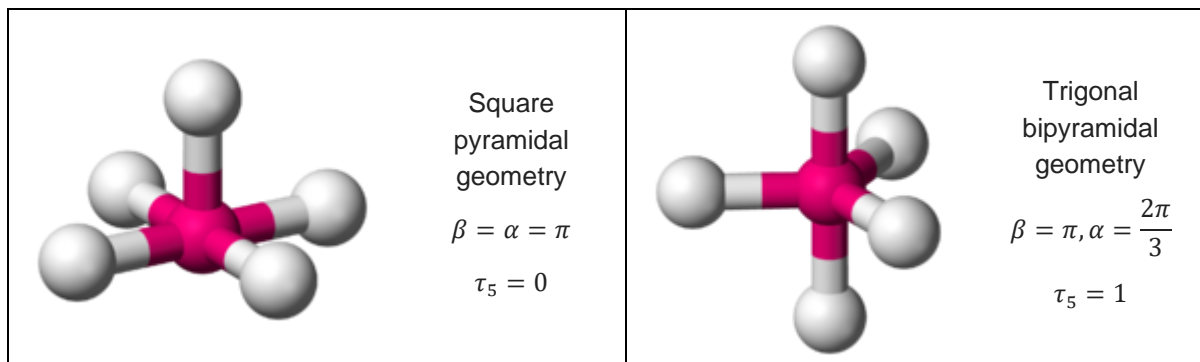


1. For five coordinate compounds, one can define a τ_5 parameter - Take the two largest valence (LML) angles in the compounds, such that $\beta > \alpha$:

$$\tau_5 = \frac{\beta - \alpha}{60^\circ}$$

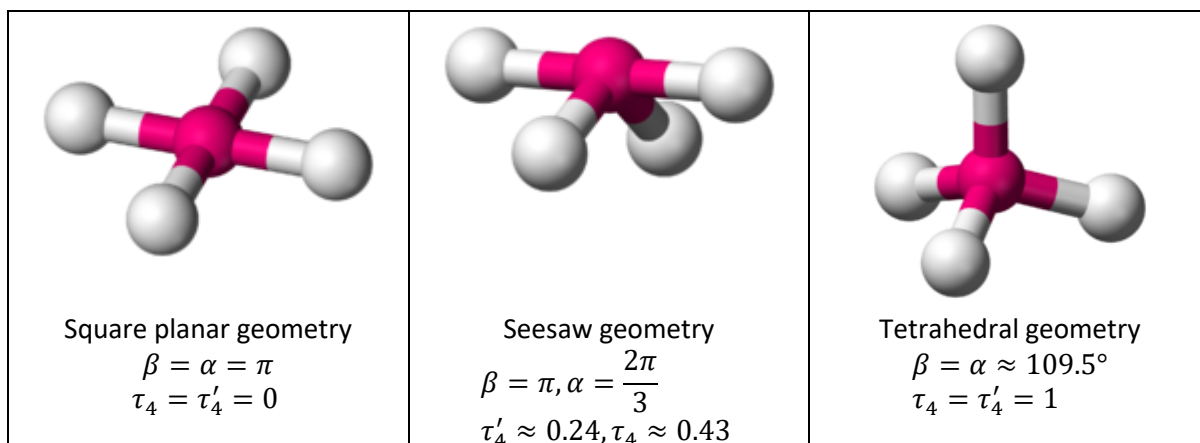
This value indicates if we are dealing with a square bipyramid ($\tau_5 = 0$), a trigonal bipyramid ($\tau_5 = 1$), or something in between, closer to one or the other.



For four coordinated compounds, the best parameter is

$$\tau'_4 = \frac{\beta - \alpha}{360^\circ - \theta} + \frac{180^\circ - \beta}{180^\circ - \theta}$$

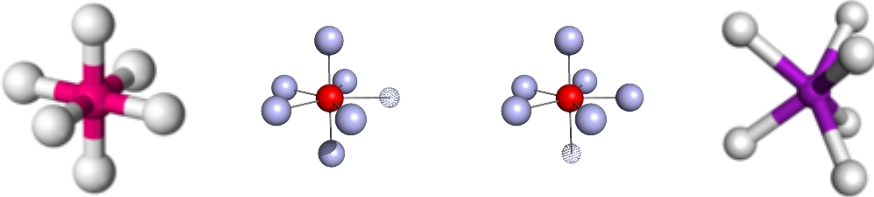
In this expression $\beta > \alpha$ are the two greatest valence angles of the coordination centre, and the interpretation is quite similar to the above one.



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

$$\tau_6 = \frac{360 - (\alpha + \beta)}{360 - 2\theta}$$

where α and β are the largest angles in the geometry and θ is $\arccos\left(-\frac{5}{7}\right)$, which is one of the LML angles in the triangular prism. This gives the following values:

	Oct ^a	PBeq ^a	PBax ^a	TriP ^a
$\alpha^{d)}$	180	180	144	135.585 ^{b)}
$\beta^{d)}$	180	144	144	135.585
τ_6	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.