Trigonal bipyramidal or square pyramidal: Another ten minute exploration.

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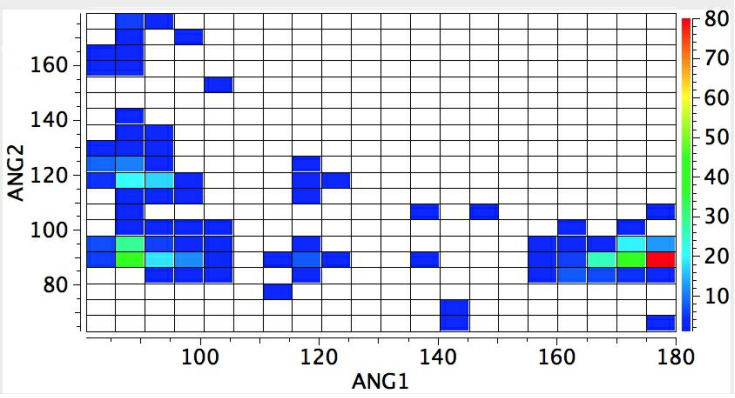
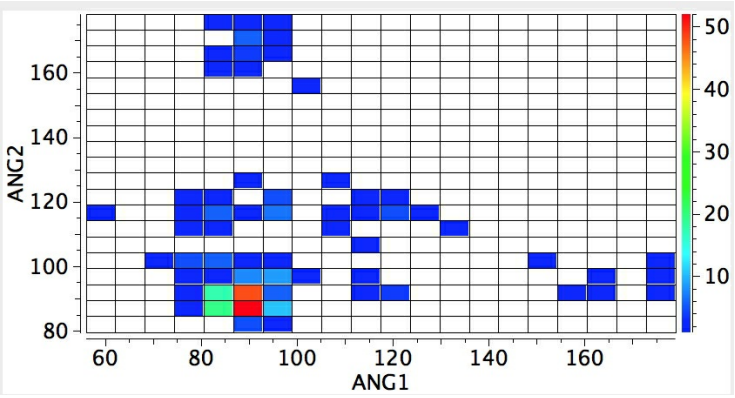
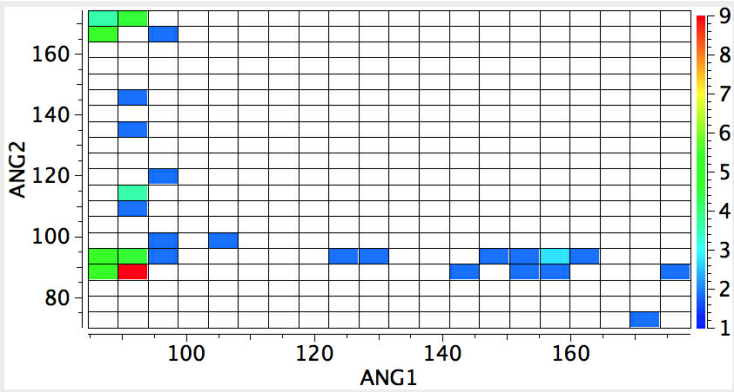
This is rather cranking the handle, but taking my previous post and altering the search definition of the crystal structure database from 4- to 5-coordinate metals, one gets the following.



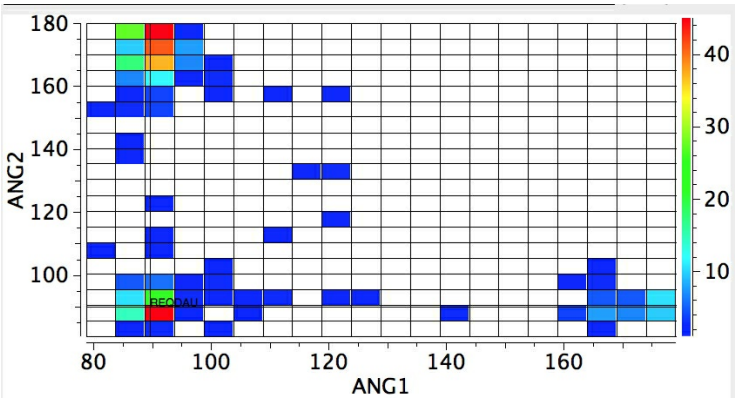
Fe …



Co …



Ni …



Cu …

Trigonal bipyramidal coordination has angles of 90, 120 and 180°. Square pyramidal has no 120° angles, and the 180° angles might be somewhat reduced. Thus the Fe and Co series have plenty of 120, whereas the Ni and Cu series hardly any. The Ni series has many 160° values. It is clearly a serious issue that attempting any correlation with the spin states is going to be a lot of really hard work (I might next do another simple search where bond lengths can be shown to very closely correlate with low/medium/high spin states). I will not be trying a more finely grained analysis of the above plots; I just wanted to point out how very simple and quick they are to generate.