

**From:** Robert Lucchese <lucchese@mail.chem.tamu.edu>  
**Subject:** mesa with C6F6 and SF6  
**Date:** August 31, 2013 9:25:47 AM CDT  
**To:** Ralph Carey <rcarey@mail.chem.tamu.edu>, Jobin Jose <jobin.jose@mail.chem.tamu.edu>

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Ralph and Jobin:

One possible solution to the problems you are having with the symmetry analysis of the orbitals in m644 is to change the parameter the program uses to decide if an eigenvalue is degenerate. The default value of smleig is 0.00001. Look at your orbital eigenvalues and make smleig small enough so that the program can distinguish between the nearly degenerate F 1s orbitals. This parameter is set using ksym= (... ,smleig=0.000001).

Please let me know if this does or does not help.

Thanks.

R. Lucchese

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