How to run PATSEE

1.) In the INS file remove all commands save TITL,CELL,ZERR,SYMM,UNIT,SFAC,HKLF,END
2.) After the UNIT command add PSEE command
3.) Run XS
4.) Rename the *.res file to *.inp
5.) Generate the fragment that you want to search for
    a. First method DATABASE
        i. Search the CSD find a similar compound SAVE as *.RES
        ii. Start XP, read the *.res file
        iii. Use the PICK command to trim the molecule to the desired fragment
        iv. Save the fragment with the ORTH command
    b. Second method : Use a modelling program to generate the fragment
        i. Save the fragment as a orthogonal text file.
6.) Edit the *.inp file and add ROTS and TRANS after the UNIT command
7.) Cut and paste the fragment into the *.inp file after the TRANS command
8.) If necessary, edit the fragment coordinates to match the SHELX format (name, type, xyz etc)
9.) Add the FRAG 1 command before the fragment and FEND after.
10.) Run XPS filename at any command prompt
11.) When complete rename the *.rep file generated by PATSEE to *.ins
12.) Run XS with the new *.ins file
13.) Proceed with normal structural workup