

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