The Center for X-Ray Crystallography
University of Florida
Written by Ashley Felts

Applying Absorption Correction

After solving structure, tending to disorder, solvents, etc.:

This details absorption correction applied according to indexed faces. The process requires a correct molecular formula.

- Open XP
    - Kill $H, note number
    - Kill $C, note number
        - Etc. so you know total molecular formula that you expect in unit cell
        - Does this include solvent?
        - Make note of the chemical formula (ex: C20 H24 N2 O3 Mn3 etc.)
- Open cmd.exe
    - Set directory to X: (or current working directory)
    - Cd 1415 (or current fiscal year folder)
    - Cd project name
- Open file mo_name_0m.p4p and edit in the chemical formula on the line:
    - CHEM ?

      By replacing the ? with the actual formula you noted above
- Cmd: xprep mo_name_0m.raw
    - Find symmetry/space group, make sure it matches what you solved
    - Go through statistics
    - Find formula/content of unit cell
    - Select [A] for absorption correction
        - Select [F] to correct based on faces
            - Psi scans if no faces
        - Check faces
        - Wavelength
        - Current absorption coefficient
        - Name of file with directional cosines should be i.e. mo_name_0m.raw
        - Copy whole of input file with updated I and sigma? Say Yes instead
            - Output file name *.abc
        - [E] exit to xprep menu
        - [F] to create shelxtl files
        - Output file name face
        - Format [s]
        - Write face.* files
- Open face.ins, solved structure .ins
    - Copy from OMIT to just before HKLF from *.ins
    - Paste to replace TREF in face.ins
- Back to CMD: xl face (no extension)
    - Check R1, wR2,GooF values
    - R1 after merging, highest peak, deepest hole

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This process details absorption correction using the program SADABS. Absorption of this type is known as correction by “psi-scans”.

- Run SADABS
  - [N] no expert mode
  - Select Laue mode (should be space group minus translational symmetry...)
  - Enter file name of data (mo_name_0m NO EXTENSION)
  - Go through defaults
    - It will go through 25 cycles
    - Look at wR2 for 1-25 to make sure it decreases
    - Accept [A]
  - SADABS part 2: defaults
  - SADABS part 3
    - Write postscript [Y], sad.eps, enter through [test]
    - [W] write hkl
    - Abc.hkl
    - Quit SADABS [Q]
- Copy *.p4p abc.p4p

- XPREP abc
- Edit abc.ins with OMIT through HKLF for TREF
- XL abc
- Cycle WGHT (full line) and refine
  - Copy bottom WGHT value to top in .res
  - Copy .res -> .ins
  - Xl
  - Watch GooF values and wR2 values (should decrease)

It is important to apply the type of correction that makes the most sense for your crystal. For example, a crystal that does not contain heavier atoms, like transition metals, is typically not treated using correction by faces.

The final .cif file should be amended to include comments about the type of correction applied, if any.

Examples include:

ABSORPTION OPTIONS

```
_exptl_absorpt_correction_type

#explanation: analytical from crystal shape
face.*  analytical
_exptl_absorpt_process_details
'based on measured indexed crystal faces, Bruker SHELXTL2014 (Sheldrick, 2014)'

#explanation: empirical from intensities
abc.*  empirical
_exptl_absorpt_process_details
'SADABS, Blessing, R.H. (1995). Acta Cryst. A51, 33-38.'

#explanation: numerical from crystal shape
hkl.*  numerical
_exptl_absorpt_process_details
'based on measured indexed crystal faces, Bruker APEX2 (Bruker, 2014)'

#explanation: psi-scan corrections
psi.*  multi-scan

#explanation: no absorption correction applied
none
```