

Mineral Physics 101: Equation of State (EoS) - Homework

Deadline: February 2nd, 2012

Goals of this problem set:

Getting familiar with EoSFit 5.2, learn about refinement strategy and how to run a refinement by using a worked example.

Reference:

Angel et al. (1997) The use of quartz as internal pressure standard in high-pressure crystallography. J. Appl. Cryst., 30, 461-466.

Project:

1. Read the reference paper. The link to a copy of the paper can be found on the course website: <http://faculty.unlv.edu/pburnley/TopPage.html>.
2. Please download the software EoSFit 5.2 from www.rossangel.com.

EoSFit 5.2 is a program to fit several different equations of state to P-V data and P-V-T data by least-squares, and to do other calculations with equations of state such as producing P-V and K-P curves from EoS parameters, doing P-V integrals, converting P-V data to f-f plots, etc..

The screenshot shows the homepage of the Ross Angel website. The browser address bar displays 'http://www.rossangel.com/home.htm'. The page features a navigation menu on the left with links to Home, Software, Crystal structures, Ross J Angel, Teaching, Miscellaneous, Contact Us, and Links. The main content area is titled 'Free software applications for crystallography' and includes a welcome message, a 'Software available for free download' section, and a 'Latest software release' section. A sidebar on the right contains a calendar for January 2012, a 'WARNING!' message, and a 'Latest software release' section.

Welcome to the "Free software applications for crystallography" website!

Crystallography is fun. Crystallography is a job. How many people in the world can state the same about their job? I am lucky that I can, and I am happy to have the great opportunity of having enough passion and skills to invest an important part of my life in doing something useful for other crystallographers, young or less, who share the same passion with me.

'Sharing' is a key word in our job. Sharing curiosity, questions, answers, thoughts, ideas. Thinking about crystallography issues from several different points of view gives me ideas to develop new software. And this arises not only from my curiosity and questions, but also and above all from that of my colleagues. It is for them that I write software applications, and it is through their collaboration, support, questions, suggestions and reports that my software can be corrected and improved: for my and their research, and fun!

Software available for free download

In this website several software applications are available for free download. Among them, a control software (SINGLE) for four-circle diffractometers, together with other specific applications to integrate, reduce and merge single-crystal X-ray intensity data. There are several applications to fit equations of state (EoS) and to perform other EoS and related calculations, and several applications to perform a number of crystallographic tasks. Just navigate around the Software pages to find further software applications.

More detailed information is available in each software application page and users' guides.
But, please first read the introduction page to software!

Hoping to keep on having feedback from users, in order to improve the existing software applications and develop new ones, I wish everybody success in research... and have fun!

Ross Angel

WARNING!
Some browsers restrict this website from running scripts. Just allow blocked content!

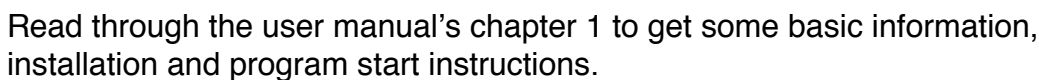
January 2012

1	2	3	4	5	6	7
8	9	10	11	12	13	14
15	16	17	18	19	20	21
22	23	24	25	26	27	28
29	30	31				

Thu 19 January 2012 9:26am

If you can not read manuals and articles from this website...
ADOBE READER

Latest software release:
Nov 2011: Strain
Download from the Software tab



Read through chapter 2 to refresh your EoS knowledge.

3. Follow the guided example in chapter 3 of the manual.

4. Send us a screenshot of your results.