



This document provides a summary of the agreed-upon protocols by which the courses associated with the pan-Canadian Computation Chemistry program will be operationalized for 2025-2026 delivery. Question about the program can be directed to Gino DiLabio (Gino.DiLabio@ubc.ca) or Alireza Sadeghifar (Alireza.Sadeghifar@ubc.ca).

1- Guidelines for PC₃ participating faculty

1. Participating faculty members will serve as the local instructor-on-record for all PC₃ courses.
2. Local instructors-on-record have the following responsibilities:
 - a. Register PC₃ courses at their university. This may be done at some institutions using existing graduate course codes.
 - b. Provide PC₃ organizers with their university's due dates for final marks at the beginning of the semester.
 - c. Ensure that PC₃ courses are scheduled at their institutions according to the delivery schedule agreed upon by the PC₃ working group.
 - d. Provide the names and email addresses of graduate students from their institution that are participating in PC₃ courses to the appropriate PC₃ instructor.
 - e. Facilitate student access to DRAC/Cedar computing resources.
 - f. Engage in mark reviews in the event that students from their institution make a grade appeal.
3. PC₃ course instructors have the following responsibilities:
 - a. For PC₃ courses involving multiple instructors, it is recommended that one instructor be identified as the course lead and take responsibility for assembling and submitting final course marks. Note that for courses with six-week modules, some institutions may require marks for two such courses.
 - b. Develop course syllabi, lectures, and assignments for portions of their course/module. All material related to the PC₃ modules will be shared with local instructors-on-record and with the PC₃ community.
 - c. Deliver courses over Zoom at the scheduled time to all students registered in their course.
 - d. Answer student questions on lecture and assignment material outside of class hours.
 - e. Mark all assigned work. Marked assignments and tests should be returned to students ideally within one week of the due date.
 - f. Provide final marks for the course module at least five working days before the end of the semester during which the course is offered.

2- Computing resources and software for course work

Students must have access to the Cedar cluster (Digital Resource Alliance of Canada (DRAC): <https://docs.alliancecan.ca/wiki/Cedar>). We are asking the local instructor-on-record to remind



students from their institution to ensure they have an account with DRAC and can use Cedar for the assignments associated with PC₃ courses. Students should work with their supervisors to obtain an account if they do not already have one.

Students will also be required to sign a license agreement to use the Gaussian-16 and Orca programs – they are encouraged to sign all necessary license agreements within the first week of the course.

Course instructors should provide additional information in their course syllabi on how to obtain access to DRAC/Cedar and ensure that the software required for the assignments related to their course are either available on Cedar or can be installed by students on their local computers. Students should be provided with instructions if they are required to install software.

Visit DRAC [User Roles to Access Resources](#) for information about access to resources based on role (Faculty, grad students, etc.). To apply for an account, see [here](#). Also, see the DRAC [Account Management Policies](#) and DRAC (/Compute Canada) [Account Renewals FAQ](#). For the available resources (including Cedar), technical documentation, and also how to request resources in the online application form visit the followings: for Cedar available software see [here](#), for technical support see [here](#), and for consultation and other inquiries see [here](#).

3- Course times and duration

1. The PC₃ group agreed that courses will be delivered as two 1.5-hour classes per week.
2. Courses will be scheduled at times of the day that will allow students from across Canada to participate. This will likely be around midday Eastern Standard/Daylight Time. We are presently finalizing the scheduling for the 2025-2026 academic year.
3. Course instructors may wish to provide student support through the following mechanisms:
 - a. PC₃ course Discord Channel. Discord access can be provided to students by the PC₃ administrators (i.e., Alireza/Gino). This is the preferred approach since it helps to build a community of practice amongst participating students. New channels will be created for students participating in PC₃ courses in 2025-2026.
 - b. E-mail.
 - c. Extra (Zoom) sessions are not recommended but students may be encouraged to self-organize discussion sessions.

4- Expectations of Participating Students

1. Students are expected to attend all classes in the modules in which they are registered. Recording of the lectures are provided to support learning.
2. Students are encouraged to get to know each other and to discuss course material together. However, assignments must be the sole work of individual students.
3. The use of artificial intelligence tools, such as ChatGPT, for assignments is prohibited.



4. Sharing of the PC₃ course materials (assignments, software instructions, lecture recordings, class discussions, Discord link, etc.) with anyone outside of the program is prohibited.
5. Students are expected to have an active account with Digital Research Alliance of Canada (DRAC) before/at the start of the course. Graduate student supervisors should have a DRAC account in place to which students will apply. If account issues arise during the PC₃ courses, they should be immediately communicated to the PC₃ course organizers (alireza.sadeghifar@ubc.ca, gino.dilabio@ubc.ca).
6. Students are required to follow the codes of conduct of their home institution, DRAC, and the PC₃ program.
7. Students are expected to communicate respectfully with the course instructors, the program coordinators, and their fellow students.
8. Student concerns that arise during the course can be addressed with the program coordinators.

5- Course/Module Offerings in 2025-2026

The Introductory module will be offered during the September-December 2025 semester and is the UBC equivalent of a 3-credit course. Advanced Module I (AMI), and Advanced Module II (AMII) are each half semester courses that will be offered during the January-April 2026 semester. See the associated syllabi for course details.

The modules will be co-taught; it is envisioned that the modules instruction for PC₃ will result in an overall lower teaching load on participants as compared to graduate teaching they may be currently doing in their own institutions.

Whether or not a PC₃ participant is teaching a PC₃ course this September, you are encouraged to participate as a local instructor-on-record (see above). Please also let students in your graduate program know about PC₃ courses.

6- Scheduling and delivery

Courses will be delivered by Zoom in two 1.5 hour meetings per week. It will be up to the module instructors how they will make use of the in-class time with the participating students (i.e., the mix of lecture and hands-on activities).

The order of delivery of the modules needs to be understood in advance for planning and scheduling your own personal time. For example, the order of delivery for the various modules is as follows:



- ✓ **Introductory module:** Richard Bowles (U. Saskatchewan), Joshua Hollett (U. Winnipeg), and Robert Szilagyi (UBC). Four weeks each.
- ✓ **AMI:** Erin Johnson (Dalhousie), Georg Schreckenbach (U. Manitoba), and Tom Woo (U. Ottawa). Two weeks each.
- ✓ **AMII:** Gino DiLabio (UBC) and Alberto Otero de la Roza (U. Oviedo) share delivery.