Summary of commands in OC

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I have made an effort to summarize all commands in OC with a short explanation. Now is the time to change or rearrange the commands to be more obvious and easy to understand. In a year or so it may be more difficult.

Please send suggestions to me as soon as possible and I may circulate them and make changes.

1 All top level commands

ABOUT	ENTER	LIST	QUIT
AMEND	EXIT	MACRO	READ
BACK	FIN	MAP	SAVE
CALCULATE	HELP	NEW	SELECT
DEBUG	HPCALC	OPTIMIZE	SET
DELETE	INFORMATION	PLOT	STEP

One restriction I have applied to commands and subcommands is that one should not need to type more than 3 characters to have a unique abbreviation.

Directly after a command the user can give some options preceeded by a slash like /output=filename or /append=filename. The output that would normally appear on the screen will instead be listed on this file with extention DAT. The output will dekete any previous content on the file but the append will add the new output at the end of the file. The output is reset to the screen after the command.

A frequent Thermo-Calc user must disable his tendency to put hyphens or underscore characters between the command and subcommand.

2 Commands without subcommands

- ABOUT the software
- BACK to calling software (or exit) after confirmation
- EXIT, terminate the software after confirmation
- FIN, terminate the software without confirmation
- HELP gives explanations about a (few) commands from the user guide

- HPCALC use the inverse polish calculator
- INFORMATION is not implemented yet
- MACRO asks for name of macro file and exectutes it
- MAP a phase diagram with 2 or more independent axis.
- NEW asks for confirmation and if so removes all data.
- OPTIMIZE asks for the number of iteration and the tries to adjust the specified model parameters to the best least square fit.
- QUIT terminates the software after confirmation

3 Commands with subcommands

Many subcommands are not implemented, I have indicated some but not all.

- AMEND should change something already entered or set. But sometimes it creates something so one should be careful if it should be an ENTER or SET command.
  - PHASE (default) asks for phase name and amends data for this phase like:
    - COMPOSITION_SET (default) adds or deletes a composition set. Composition sets are needed for miscibility gaps when a phase can be stable with two or more compositions. A composition set can be identified with a hash symbol "#" followed by a number or by a user specified prefix or suffix. Deleting a set will always be the one with the highest number. When adding a set the user can provide a prefix and suffix and the default constitution for this set.
    - MAGNETIC_CONTRIB adds an Inden-Hillert magnetic model.
    - DISORDERED_FRACS adds a disordered fraction set for an ordered phase. This replaces AMEND ... DISORDERED_PART in Thermo-Calc.
    - GLAS_TRANSITION adds a glas transition model (not implemented).
    - QUIT You did not want to amend anything.
    - DEFAULT_CONSTIT amends the default constitution for a composition set of the phase. Same as SET PHASE "name" DEFAULT_CONSTITU.
    - DEBYE_CP_MODEL adds a Debye Cp model (not implemented).
    - EINSTEIN_CP_MDL adds a Einstein Cp model (not implemented).
    - INDEN_WEI_MAGMOD adds a magnetic model according to Wei (not implemented).

    * ELASTIC_MODEL_A adds an elastic model (not implemented). Note the LIST MODEL_PARAM_ID how to enter T, P and composition dependent elasic constants and lattice parameters.
  - ALL_OPTIM_COEFF the user can rescale or recover values of coefficients that are assessed.
  - BIBLIOGRAPHY asks for a bibliographic id and amends its text.
  - COMPONENTS changes the set of components (not implemented).
  - CONSTITUTION asks for a phase and the user can amend the amount and current constitution of a phase. I have put this here and not as part of AMEND PHASE to avoid confusion with adding a composition set.
  - CP_MODEL not implemented and probably redundant.
  - ELEMENT amends data for an element (not implemented).
  - EQUILIBRIUM not implemented yet
  - GENERAL can name of current equilibrium, the user can specify if he is a beginner (the software can provide more help (not implemented)), or expert, if global gridminimizer should be used and if it can merge composition sets, if composition sets can be created automatically and if redundant composition set can be deleted after an equilibrium calculation. The latter questions are mainly interesting for debugging.
  - PARAMETER amends a parameter expression for a phase (not implemented).
  - QUIT you did not want to amend anything
  - SPECIES amends data for a species (not implemented).
  - SYMBOL the user can specify if the symbol can only be calculated when explicitly named (usually all symbols are evaluated when any symbol is evaluated as they can depend on each other). This is needed for symbols used as conditions.

    The user can also specify that a symbol should be local to a specific equilibrium. In this way one can store the value of a symbol from one quilibrium and calculate differences with respect to other equilibria.

    The value of symbols that are constants can be changed
  - TPFUN_SYMBOL amends a TPfun expression.

- CALCULATE various things like:
  - EQUILIBRIUM (default) is the normal equilibrium calculation command which first calls the grid minimizer (if the conditions allow) and then the iterative minimizer.
  - ALL_QUILIBRIA all equilibra speficied by a SET RANGE command and have non-zero weight are calculated.

  - GLOBAL_GRIDMIN Only the grid minimizer is called to find the gridpoints that reperesent the lowest Gibbs energy. These are normally used by the iterative minimizer to find the real equilibrium. If followed by COMPUTE NO_GRDMIN one will have the same result as COMPUTE EQUILIBRIUM.
  - NO_GLOBAL calculates the equilibrium for the current set of conditions starting from the current set of stable phases and their constitutions. No grid minimizer called.
  - PHASE ask for phase name, amount and constitution and at current T and P calculates either:
    * ONLY_G Gibbs energy and first and second derivatives with respect to T and P.
    * G_AND_DGDY calculates also all first derivatives with respect to the phase constituents.
    * ALL_DERIVATIVES Also all second derivatives with respect to the phase constituents.
    * CONSTITUTION_ADJUST will calculate G and all derivatives after adjusting the constitution of the phase to have the minimum Gibbs energy for the same overall composition as the original constitution. It is only interesting when one or more components are parts of several constituents.
  - QUIT if you did not really want to calculate anything.
  - SYMBOL Calculate the value of one or all symbols at the current equilibrium.
  - TPFUN_SYMBOLS all TP functions values and their first and second derivatives with respect to T and P (6 values).
  - TRANSITION asks for a phase to be stable with zero amount and a condition to be released to calculates the equilibrium. The phase must not have the FIX status. After the calculation the phase is set to be entered and the released condition set to the calculated value. If calculation fails the status is not reset (sorry I have not had time to do all). No grid minimizer called.

- DEBUG Nothing of this works
  - FREE_LISTS
  - STOP_ON_ERROR
  - ELASTICITY

- DELETE Only composition sets can be deleted. To delete a parameter you can amend its expression to be zero.
  - PHASE (default) but not allowed
  - ELEMENTS not allowed

  - SPECIES not allowed
  - QUIT you did not want to delete anything
  - COMPOSITION_SET The highest set is deleted (one cannot delete all).
  - EQUILIBRIUM deletets the equilibria with the specified name. Fragile, handle with care.

- ENTER is the main command to enter data interactivly. Note that in most cases data are read from a TDB file.
  - SYMBOL (default) name and expression of a state variable function.
  - BIBLIOGRAPHY enter a bibligraphic reference id and text.
  - COMMENT a text line as added to the current equilibrium. Useful to specify the source if experimental data for example.
  - CONSTITUTION to enter the constitution of a phase (same as AMEND CONSTITUTION).
  - COPY_OF_EQUILIB the current equilibrium is coped to a new one with a name specified by the user.
  - ELEMENT an element with data.
  - EQUILIBRIUM an equilibrium record with the specified name is created. Each equilibrium record has an independent set of conditions. Will be used for assessments and is already used to store node points during step and map.
  - EXPERIMENT for assessments.
  - MANY_EQUILIBRIA allows the user to enter many equilibria of the same type. Useful for assessments. There is a shorthand way of specifying the phase status (by default all phases are suspended) and the conditions and experimental data. It is possible also to specify comments, symbols that should be calculated and state variables and properties that should be listed.
  - OPTIMIZE_COEFF creates symbols for coefficients to be optimized. They have the name A00 to Aij where ij is one less than the value specified by the user. Maximum 100.
  - PARAMETER the expression of a parameter of a phase. The phase, the constituent array and degree must be specified.
  - PHASE a phase with sublattices, site ratios and constituents. The parameters are entered individually with ENTER PARAMETER.
  - QUIT you did not want to enter anything.
  - SPECIES a species with name and stochiometry. Its name must be unique but one can have several with the same stoichiometry.
  - TPFUN_SYMBOL The name and expression of a function of T and P that can be used in parameters.

- LIST of many things ...

  Note the possibility to direct output to a file using /output=filename or /append=filename directly after the basic command, as mentioned in the beginning.

  - RESULTS (default) from an equilibrium calculation. the program asks for a number how to format the phase information.
    1. means stable phases and composition in mole fractions in value order
    2. means stable phases and composition in mole fractions and constitution
    3. means stable phases and composition in mole fractions and alphabetical order??
    4. means stable phases and composition in mass fractions in value order
    5. means stable phases and composition in mass fractions in alphabetical order??
    6. means stable phases and composition in mole fractions and constitution
    7. means all phases and composition in mass fractions
    8. means all phases and composition in mole fractions and constitutions
    9. means all phases and composition in mole fractions and alphabetical order
  - AXIS lists current axis set by the user.
  - BIBLIOGRAPHY lists bibliographic text for specific id or all.
  - CONDITIONS lists all conditions in current equilibrium.
  - DATA lists all parameters on different devices and ways:
    * SCREEN (default) Writes all parameters for all phases on the screen including the bibliographic information.
    * MACRO Writes all parameters on file as a macro file (not implemented).
    * LATEX Writes all parameters on file as a LaTeX file (not implemented).
    * ODB Writes all parameters on file in the OC speccific TDB format.
    * TDB Writes all parameters on file in Thermo-Calc TDB format.
  - EQUILIBRIA lists all entered equilibria with name and number (no results).
  - LINE_EQUILIBRIA lists all equilibra stored during STEP or MAP. With the SET ADVANCED command one can copy one of these to the current equilibrium.
  - MODEL_PARAM_ID lists all implemented model parameter identifiers like G, TC, BMAGN, elastic constants etc. that can depend on T, P and constitution of a phase. The use of such parameters require implementation of the model in the software.
  - OPTIMIZATION list results from an optimization.
  - PARAMETER lists the expression for a single parameter.
  - PHASE asks for phase name and then lists for option
    * CONSTITUTION (DEFAULT) lists constitution for this phase.

    - * DATA lists parameter for this phase (no bibliography).
    - * MODEL lists some model information for this phase.
  - QUIT You do not want to list anything.
  - SHORT
    - * A writes one line for all elements, species and phases.
    - * P writes one line for all phases sorted with stable first, then max 10 entered phases in decreasing stability, finally the dormant in decreasing stability.
  - STATE_VARIABLES asks for state variable symbol and lists it value. Can also be used for the current value of model parameters as Curie temperature (TC(BCC), etc.

    I will try to merge list state_variables and compute symbol to a SHOW command
  - SYMBOLS lists all entered state variable symbols (same in all equilibria). To calculate the value of a symbol use CALCULATE.
  - TPFUN_SYMBOLS lists one or all TP function symbols and expressions (same in all equilibria).

- PLOT asks for state variables or symbols for x and y axis and after that the user can plot directly or change anything in the submenu below.

  OC generates a command file for GNUPLOT and a data file with the values to plot and then executes this in a separate shell. The user can edit the command file to add options and execute it again inside gnuplot. But beware not to overwrite the files you want to edit. There are 10 colors for the lines to plot. If more than 10 lines to plot the colors are repeated cyclically.

  OC keeps the previous values set of all options set (except the scaling of an axis with a new variable and the output file which is always reset to the default "ocgnu") unless an option is explicitly changed.

  - RENDER (default) finally plot when all options set.
  - GIBBS_TRIANGLE set diagram to be a Gibbs triangle (not implemented).
  - GRAPHICS_FORMAT set type of terminal (P for postscript, G for gif). You will also be asked for output file.
  - OUTPUT_FILE set name of plot file (default is ocgnu.dat).
  - POSITION_OF_KEYS select position of the labels (identification) of the lines in the plot. The lables can be placed inside/outside of the plot, to the left/center/right and top/bottom. See the explanation of "set key" in GNUPLOT.
  - QUIT you do not want to plot.
  - TITLE set title of plot.

  - XRANGE set plot range (default or min and max) on x axis.
  - YRANGE set plot range (default or min and max) on y axis.
  - XTEXT set text on x axis.
  - YTEXT set text on y axis.

    More options will be added when I understand GNUPLOT better

- READ At present only TDB and UNFORMATTED implemented.
  - TDB (default) an unencrypted TDB file can be read. Many TYPE_DEFS are not handelled correctly and warning are given. For partitioned phases you may have to edit the parameters.
  - DIRECT will save results from STEP and MAP on a random acess file (not implemented).
  - QUIT you did not want to read anything.
  - UNFORMATTED an unformatted file with model parameters and results for a single equilibrium calculation. This is very fragile as any change in the data structure may make it impossible to read.
- SAVE The only save option (partially) implemented is unformatted.
  - UNFORMATTED (default) A file is written with unformatted data for all thermodynamic data and conditions and results for a single equilibrium. There is no guarantee an unformatted file will be readable in a later version of OC.
  - DIRECT not implemeted yet (for STEP and MAP results).
  - QUIT do not save anything.
  - TDB the data will be written in the TDB format on a file. Same as the LIST DATA TDB command.
- SELECT a few things.
  - EQUILIBRIUM (default) change the current equilibrium to the selected one (number or name or next or previous).
  - GRAPHICS there is only one (GNUPLOT)
  - LANGUAGE there is only one (English).
  - MINIMIZER there is only one (HMS).
  - OPTIMIZER there is only one (LMDIF).
- SET can be used for many things. The most important is conditions.
  - CONDITION (default) the state variable and value of a condition. Only single values are allowed, expressions not yet implemented.

- ADVANCED This command for very special things.
  - EQUILIB_TRANSF transfer an equilibrium calculated along a line in STEP or MAP to current equilibrium.
    this is probably the most awkward command of all. But I do not want to have a TRANSFER or COPY command on the top level as that will certainly be misunderstood and misused
  - QUIT you did not want to set anything advanced.
- AS_START_EQUILIB use current equilibrium as start for step or map. Not necessary if there is only one start equilibrium.
- AXIS axis "number" to an independent variable (must be a condition).
- BIT some global bits can be set. Never change these unless you are an expert.
  - 0 set if you are a beginner
  - 1 set if you are an occational user
  - 2 set if you are an expert
  - 3 set if gridminimizer not allowed
  - 4 set if gridminimizer must not merge comp.sets
  - 5 set if these is no data
  - 6 set if there is no phases
  - 7 set if not allowed to create comp.sets automatically
  - 8 set if not allowed to delete comp.sets automatically
  - 9 set if data changed since last save
  - 10 set if verbose'/'11 set if explicit verbose
  - 12 set if very silent
  - 13 set if no cleanup after an equilibrium calculation
  - 14 set if dense grid in grid minimizer
  - 15 set if parallel execution not allowed
- ECHO echo of the input from macro files on the screen.
- FIXED_COEFF to set an optimizing coefficient to a fixed value.
- GRAPHICS_OUTPUT ??
- INPUT_AMOUNTS amount of species. These will be added together and used for conditions of the components.
- INTERACTIVE at the end of macro files.
- LEVEL I am not sure what this was intended for.
- LOG_FILE the name of a file with a copy of all input and defaults.
- NUMERIC_OPTIONS maximum number of iterations (default 500) and convergence limit (default 10^{-6}).

- OPTIMIZING_CONFITION some criteria for the least square routine cab be set.
- PHASE the user must specify a phase name and can then ...
  - STATUS (default) the status of a single phase, or all using an asterisk "*", can be set. See also SET STATUS PHASE with a more flexible way to specify phases.
  - DEFAULT_CONSTITU the default constitution of the phase can be set. Same as AMEND PHASE name DEFAULT_CONSTITU.
  - AMOUNT the amount of the phase (redundant).
  - QUIT nothing is set for the phase.
  - BITS some special bits for a phase can be set. At present there is no way to "UNSET" these bits ... so be careful.
    - QUIT (default) no bit is changed.
    - FCC_PERMUTATIONS to indicate 4 sublattice fcc or hcp permutations. Only one parameter stored for each unique permutatation. Must be set before any parameters are entered.
    - BCC_PERMUTATIONS to indicate 4 sublattice bcc permutations. Must be set before any parameters are entered (when implemented).
    - IONIC_LIQUID_MDL to indicate ionic liquid model. A phase with the ionic liquid model that is entered interactivly must currently have the name ionic_liquid and this bit is automatically set. If read from a TDB file the :Y after the phase name assignes this model. Setting this bit interactivly has no function at present.
    - AQUEOUS_MODEL to indicate aqueus model (not impemented).
    - QUASICHEMICAL to indicate quasichemical model (not implemented).
    - FCC_CVM_TETRADRN to indicate CVM fcc tetrahedon model (not implemented).
    - FACT_QUASICHEMCL to indicate FACT quasichemicval model (not implemented).
    - NO_AUTO_COMP_SET to prevent automatic creations of composition sets for this phase. One can forbid creating automatic composition sets (by the grid minimizer) for all phases with the AMEND GENERAL command.
- QUIT you did not want to set anything.
- RANGE_EXP_EQUIL the first and last equilibrium number of equilibria with experiments. Can also be used for equilibria that shoyld be calculated with CALCULATE MANY.
- REFERENCE_STATE the reference state of a component. The phase, T and P must be specified. The phase must exist with the component as its only component. When the phase can exist with the component in different ways, like O in a gas can be O, O_2 or O_3 the most stable is selected.

- SCALED_COEFF a min and max for an optimizing coefficient can be set.
- STATUS
  - PHASE (default) one or more phases can be set as suspended, dormant, entered or fixed. You can use * to mean all phases, *S for all suspended, *D for all dormant and *E for all entered and *U for all entered and unstable. The list of phases is terminated by an equal sign "=" or an empty line.
    If the new status is not already given after the equal sign it is asked for. If the new status is entered or fixed the amount is asked for.
  - ELEMENT an element can be entered or suspended.
  - SPECIES a species can be entered or suspended.
  - CONSTITUENT not implemented.
- UNITS like energy Joule/cal or mass kg/lb ... but not implemented yet.
- VARIABLE_COEFF a start value for an optimizing f´coefficent is set.
- VERBOSE the software will write extra output.
- WEIGHT of an equilibria with experiments is set. If zero the equilibrium will be ignored. An asterisk, *, means all equilibria and abbreviations of equilibrium names can be used.

- STEP is used to calculate along a single independent axis variable.
  - NORMAL (default) follow the axis variable from low to high limit.
  - CONDITIONAL follow the axis variable and update s symbol after each step (to be used for Scheil-Gulliver simulations, not yet implemented).
  - QUIT do not step.
  - SEPARATE calculate each phase separately.

That is all. You are welcome to suggest more options or rearrangements of the commands that seems more easy or obvious.