CUTOFF

CUTOFF was created by IHW at the University of Bath, UK. Its function is to create a subset Hessian from an input structure with a full Hessian, allowing the user to select the atoms to be retained, the rest being excluded. The output from program CUTOFF is used as input for program UJISO, available elsewhere at the following Github repository: https://github.com/pbw20/SULISO).

CUTOFF is written in Fortran90, with some elements of earlier versions, but compiles fluidly under standard GNU compilers (gfortran…).

The aim of this user guide is to gently introduce the individual to the functionalities of CUTOFF and provide explicit descriptions of the input and output one can expect from standard CUTOFF runs. We will begin by discussing the format of the input, suggesting possible edits to the source code, which is available from the SULISO_source repository on Github: https://github.com/pbw20/SULISO_source

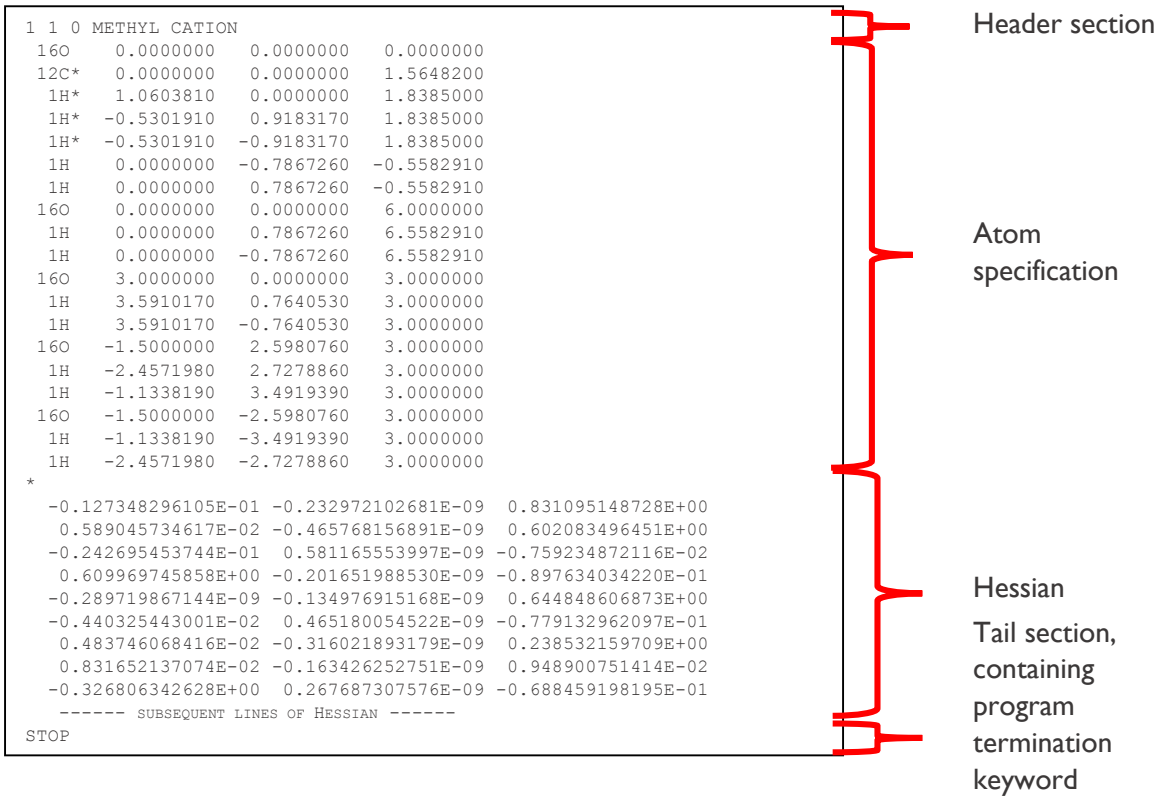

Figure 1. Sample input file for CUTOFF. In the interest of space, only the first few lines of the Hessian are included, with the "------ SUBSEQUENT LINES OF HESSIAN ------" line indicating their original position.

Overview of CUTOFF input

1. Header section, line 1: (FORMAT 3I2,74A)

   The symmetry number (in this case, 1) and charge are included, followed by the number of frequencies to be input if instead of Hessian.
   The title follows (74A): this can be anything at all and does not enter into the calculation routines of the program. Most often used as an additional descriptor for the file or calculation.

2. Coordinate input, line 2 – line 2 + *n*, where *n* is the number of atoms: (FORMAT A4,A1, 3F12.8)

   n atoms and their Cartesian coordinates are input as the isotopologues, followed by a space, followed by the *x*, *y*, and *z* coordinates in the format 3F12.7. The following isotopologues are currently accepted, although the nature of CUTOFF allows editing and inclusion of any entity by editing the source code:

   1H , 2H , 3H , 12C , 13C , 14C , 14N , 15N , 16O , 17O , 18O , F , 32S , 34S , 35CL, 37CL , 6LI , 7LI , 9BE , 10B , 11B , SI , P , 79BR , 81BR , NA , SP , MG , AL , CL , K , CA , ZN , BR , RB , I , CS , B , H , C , N , O , S , HE , NE , AR , KR , 33S , 36S , 11C

   The nature of the A1 format specification is inherently important in this program. This is the slot where the atoms to be retained are identified by asterisks (*), one per atom, to be placed directly after the atom label. Atoms without an asterisk are ignored by cutoff and their corresponding rows and columns in the Hessian are excluded from the output file.

3. Coordinate-Hessian separation line, line 3 + *n* : (FORMAT A5)

   Consists of an asterisk (*) followed by four spaces, to separate the coordinate input from the Hessian.

4. Hessian input lines, line 3 + *n* – line *q*, where q = number of lines before Hessian section (6) + number of atoms (*n*), + number of lines of Hessian (*m)*: (FORMAT: 1X, 3E20.16)

   The number of lines of Hessian can be calculated based on the three column input being specified. Where:

   $$\text{Number of lines of Hessian, } m = \frac{3n}{2} \times \frac{3n+1}{3}$$

   Therefore the number of lines of Hessian output from a calculation can be used to verify the reasonableness of the input, by comparing this with the number of atoms using the formula above.

5. Final line: (FORMAT A4)

   The final line of the program consists of the word STOP, followed by a line break, in order to inform the program that no more input remains to be read.

Overview of CUTOFF output

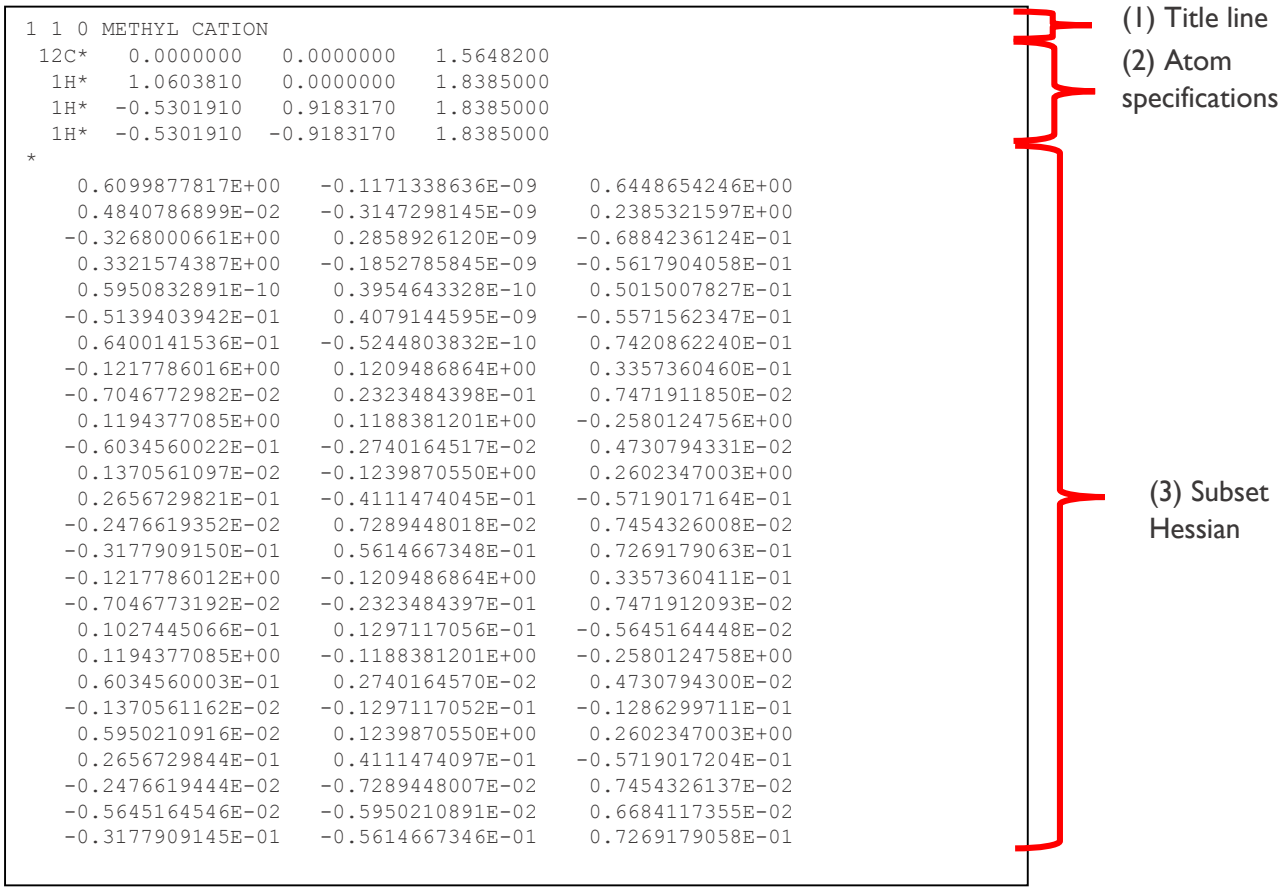

Figure 2. CUTOFF output generated from the file in Figure 1.

1. CUTOFF output begins by printing the title line with symmetry number, degeneracy and the miscellaneous title characters chosen by the user.

2. The new subset molecule is printed by atomic symbol and Cartesian coordinates

3. The subset Hessian is printed out, with the rows and columns present corresponding to the atoms printed above.

CUTOFF Troubleshooting guide

There are a number of errors that users can come across, which will hopefully decrease in number as they familiarise themselves with the code. The most common of these are input errors. Luckily, the program will inform the user within the UNIX environment of the last read format and line number in the fortran source code, and therefore a likely area linking to the error. Throughout this manual, the formats of input have been specified to allow the user easy identification of the areas which require specific types. This should be the first reference point in the case of incomplete termination.

One error that has been noted is the format of certain coordinate/Hessian outputs from electronic structure codes. Some codes simply print out the coordinates, followed directly by the Hessian. However, sometimes the gradient is printed following the coordinates and preceding the Hessian. This consists of *n* lines of a similar format to the Hessian, where *n* is the number of atoms in the structure. This is often noticed upon processing, where erroneous frequencies are printed from the program and the input needs to be re-inspected. The simplest solution is to use the equation in Part 4 of the *Overview of CUTOFF input* to deduce the expected number of lines of Hessian, and a program such as Notepad++ with a line count to identify if lines of gradient are present. When located, these can simply be deleted from the input and the programs rerun, which should fix the errors.